# Perfume and Flavor Chemicals

## (Aroma Chemicals)

## I

*By*

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To

RUTGERS UNIVERSITY

THE STATE UNIVERSITY OF NEW JERSEY

For pioneering the first college programs in perfumery, flavor technique, essential oils and raw materials through the University Extension Division and The College of Pharmacy.

# Perfume and Flavor Chemicals

## (Aroma Chemicals)

A perfumer-flavorist's practical description of most of the commercially available perfume and flavor chemicals, with their chemical structure and practical physical data, appearance, odor and flavor type, reported and suggested uses, production and evaluation, with literature references for further details and study.

*In two volumes:*

VOLUME ONE
Monographs No. 1 to 1790 (A through J)

VOLUME TWO
Monographs No. 1791 to 3102 (K through Z)

# Perfume and Flavor Chemicals

## (Aroma Chemicals)

## VOLUME ONE

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Monographs No. 1 to 1790

(Letters A through J)

# Preface

This work is the collated results of experienced and collected information and notes, private search, and experiments carried out and accumulated over a period of 34 years.

Increasing emphasis has been placed upon the results from the explosive growth of the perfume and flavor chemical industry, and from advanced analytical methods introduced during the past 12 to 15 years.

This book was written and edited for the chief purpose of supplying comprehensive, practical and yet brief information, readable not only by perfumers and flavorists in the fragrance and flavor industries, but also by chemists and non-chemists in related fields and industries. Its chemical information includes quotations from very recent chemical publications and may therefore not always be news to the alert and expert chemist.

The chemical nomenclature in this work is a compromise between the modern and internationally accepted nomenclature on one side, and the actual, practical perfumery and flavor language on the other side. The author refers the reader to the "Explanations to Index" appearing just before the index in the back of volume No. Two.

The use of Capital letters may be unconventional, but it is intentional, partly for purposes of "speed-reading," partly for increased distinction.

The occurrence in Nature of various chemicals is generally not mentioned in this work. For two reasons: It is beyond the scope of this work to describe "all known odorous chemicals and all components identified in fragrance materials, flavor materials, food, etc.". This type of information is comprehensively covered in recent special literature, well elucidated and frequently brought up to date. It is, furthermore, in the author's opinion, confusing to mention the non-existence in Nature of a chemical, when chances are that this chemical may be identified in a natural product within the next few years or so. This has happened to scores, if not hundreds of perfume and flavor chemicals since 1950.

Although this work was intended to be a companion to the first book "Perfume and Flavor Materials of Natural Origin", published in 1961, the author is quite aware that a book on chemicals cannot be absolutely up to date or complete - at the date of publication. Final proofreading and cleantyping of the completed manuscript covered a period of almost two years, and editing was "closed" by December 31st, 1968. Thanks to the high accuracy and exceptional workspeed of the printers, the book could still be published in 1969.

The appearance on the market of new chemicals, including Aroma-chemicals, is a continuous and growing feature. Although probably more than 95% of the newly developed fragrance and flavor research chemicals never reach the shelves of the perfume and flavor laboratories, the annual number of new additions to the perfumer's "palette" is enormous.

Information about the production, location and volume of Natural materials is accessible, while similar information about chemicals is often inaccessible or deliberately kept at a "discrete" level, partly for ethical reasons, partly for other reasons.

The author takes this opportunity of appealing to readers who may wish to write to the author for additional information, that - as a rule - such information cannot be supplied, for ethical reasons.

Vast differences in "company policy" are also responsible for the fact that certain products are mentioned with ample information and data, while other chemicals are included with very scanty information or not mentioned at all. The author has avoided mention of all such perfume and flavor chemicals for which only a trade name and no information on chemical identity has been available.

It is the author's hope that this work, with all its information, including its opinions and its errors, may serve as another stepping stone for future progress and improvement of the quality and quantity of perfume and flavor chemicals.

By challenging those who have specific and superior knowledge on one or many of these subjects, our industry should be able to continuously improve such future publications.

*07042 U.S.A.*
*April 1969*

STEFFEN ARCTANDER

# Odor Descriptions

The materials described in these monographs have been studied and evaluated on conventional type perfume blotters, repeatedly and over a sufficiently long period of time, so that characteristic terminal notes - or the characteristic absence of same - may be reported in the odor descriptions.

A chemist may find it peculiar, that a chemical can display a variety of odors, and our theory of olfaction should also tell us that - most conceivably - a single chemical should only display one definite odor.

However, perfume chemicals are rarely used in such a state of chemical purity, that they are absolutely free from other components. The odor of these components - impurities, etc. - may appear before or after the odor of the proper material. The more annoying impurities will blend with the odor of the material to produce a complex odor, sometimes very consistent, but usually distinctly different from the odor of the pure material. Finally, there are impurities which do not influence the odor of the perfume chemical in a perceptible manner.

In an attempt to reduce the unquestionable disadvantage of a highly subjective odor (and flavor) description, the author has made extensive use of personal notes, made during 11 years of evening lecturing at Rutgers University, The State University of New Jersey. More than 350 students have attended classes. Many of the students have given very useful comments, odor and flavor descriptions. By including part of such descriptions or terms with some of the author's personal notes, he feels that a more reasonable and practical odor (and flavor) description has been achieved. This may explain why the odors of certain chemicals are described using a great variety of words.

Odor descriptions are occasionally quoted from literature, particularly if they are strongly inconsistent with the author's subjective odor or flavor descriptions.

# Flavor Descriptions

Flavor chemicals have been studied and evaluated in aqueous solution, usually with a modest amount of sugar (6 to 9%), occasionally with a food acid, and - for most Vanilla flavor chemicals, etc. - in sweetened ice-cold milk. Evaluations were always carried out against an unflavored medium. See also "Abbreviations" for explanation of the term "ppm."

# G.R.A.S.

When it is stated that a material is NOT listed as G.R.A.S. by the F.R. or the F.E.M.A., the author will make the reservation that such statement means "at the time of writing this monograph". It is very probable, that certain materials may be approved or considered as G.R.A.S. at a later date, thus amending the author's statement.

# Acknowledgements

Since the work on this book dates back as far as 1935, when the author started collecting information on perfume and flavor chemicals, it would be virtually impossible to thank all the individual persons, institutions, commercial or non-profit organizations, etc. who have contributed to the completion of this work.

Long periods of events or other work prevented or delayed the compilation of notes, while new information on known chemicals often completely cancelled or outdated previous notes, so that actually the book had to be re-written as late as possible and as quickly as possible.

Rutgers University, The State University of New Jersey, has been most helpful to the author in making more authoritative contacts and procuring expert comments.

Students at the Perfume and Flavor Materials courses at Rutgers University, The State University of New Jersey, and at The University of Maryland, have contributed greatly to the broadening of odor and flavor descriptions in this work, thus reducing the drawback of very subjective and personal descriptions from the author.

The perfume and flavor chemical industry has supported the author with samples, often of non-commercial or experimental, new chemicals and information on same. The author sincerely wishes that he could mention names of particularly co-operative companies.

Colleagues in the perfume and flavor industry have encouraged the author in completing this work, which at times appeared to be insurmountable.

Technical periodicals have supplied the author with much useful and recent information, and the author takes this opportunity of thanking all those who are not specifically mentioned in the literature reference index.

Finally, the author wishes to express his thanks to the printers in Copenhagen for making it possible to complete this work with exceptional accuracy and speed, virtues of paramount importance in making this type of handbook particularly valuable.

Since this book is an entirely personal undertaking, the author will be fully responsible not only for the useful information in the book, but also for its possible errors, omissions and defaults. As mentioned briefly in the latter part of the Preface, many omissions are intentional and ethically necessary.

# Abbreviations

B.P. = Boiling point at atmospheric pressure, in Centigrades. Boiling points higher than 280°C are given "approximately".

M.P. = Melting point in Centigrades.

Sp.Gr. = Specific Gravity at 20°C. Figures are given approximately and with no reference to temperature, since this accuracy is sufficient for the perfumer's or the flavorist's daily work. Literature references will provide more exact data.

Soluble: "15% soluble in alcohol" means that the material is soluble in Ethyl alcohol at the rate of 15 grams material plus 85 grams alcohol at room temperature.

"Slightly soluble" refers to a physically poor solubility which, however, is sufficient to provide odor or taste experiments.

"Very slightly soluble" usually means "soluble at the rate of less than 0.1% in the solvent at room temperature", but still sufficient to produce odor or flavor for evaluation.

Prod. = produced (... method).

ppm. = Parts per Million. A term used also by flavorists to indicate the concentration of flavors in the flavor compositions or (more commonly) in the finished consumer product.

Figures given in this work indicate concentration in the *functional product, i.e., the finished consumer product, food, beverage, candy*, etc. - unless otherwise stated.

The term "ppm" is almost exclusively applied to flavors, very rarely to fragrances.

One percent is equivalent to Ten Thousand Parts per Million. "Traces" refers to concentrations of a few ppm or less.

Alcohol = Ethyl alcohol (95% by volume unless otherwise stated).

G.R.A.S. = Generally Recognized As Safe. An indication that the material has not been banned from use in food products in the U.S.A.

A material may be recognized as safe by an expert flavorist panel (e.g. of the F.E.M.A.) and yet not be adopted in the G.R.A.S. list issued by the F.R. (Federal Register). However, the authorities will normally agree on the findings and results from the expert panel.

The G.R.A.S. list is therefore never ending, continuously updated with amendments, many additions, but also with new bans on chemicals formerly approved, or with limitations of use for certain chemicals.

F.E.M.A. = Flavoring Extract Manufacturer's Association (U.S.A.). A panel of this association is responsible for the list of G.R.A.S. materials, see also literature No. 162.

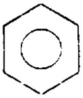
F.D.A. = Food and Drug Administration (U.S.A.)

F.R. = Federal Register (U.S.A.) whose responsibility includes the G.R.A.S. list and its continuous amendments.

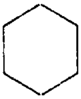
F.C.C. = Food Chemicals Codes - see literature No. 154.

C.N.S. = Central Nervous System (human).

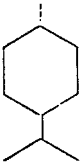
The following chemical structures are used in simplified form:



(saturated)
Cyclohexane ring



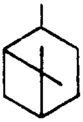
(unsaturated)
Benzene nucleus



← (Methyl group)

*para*-Menthane skeleton

← (*iso*-Propyl group)



Pinane skeleton

# Key to the use of this work

The 3,102 monographs in this work are listed, using strict alphabetic order of title names. There is no pagination, but the index will refer the reader to the wanted monograph through the use of numerous synonyms.

Materials under title names A through J (monograph numbers 1-1790) are listed in volume No. One, while materials under title names K through Z (monograph numbers 1791-3102) are listed in volume No. Two. The index is included at the end of volume No. Two.

It is therefore advisable to look up in the index any name before looking directly in the monographs. The title name is not always the most common to the user, but the synonyms in the index will refer to the proper monograph number, and subsequently to the proper volume and location of the monograph.

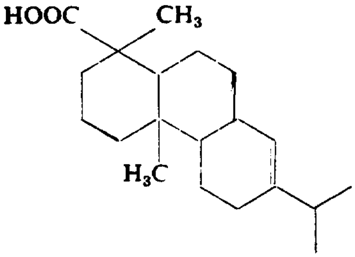
The preface in the beginning of volume No. One, and the "Explanation to Index" at the end of volume No. Two, as well as the radical synonym list will give additional information helpful to quick use of this reference work.

Prefixes may or may not be alphabetized. "Explanations to Index" will explain this in accordance with modern chemical literature and conventions generally agreed upon.

Not all trade names are included in the index, and the reader is kindly asked to search primarily under chemical names, since the extended use of trade names could easily lead to a preference for certain manufacturers, who make a policy of offering all or most of their chemicals under trade names, even when the material is actually well-known under a chemical name.

# 1: ABIETIC ACID

Sylvic acid.
Dimethyl-*iso*-propyl-decahydrophenanthrene carboxylic acid.



$C_{20}H_{30}O_2 = 302.46$

The pure material is almost white, crystalline plates or powder. M.P. 174-182°C.

Lower grade commercial material is usually off-white or pale straw-colored, granular crystals or conglomerated mass with much lower melting point.

Insoluble in water, soluble in alcohol and oils. Also soluble in aqueous solution of Sodium hydroxide.

The pure material is virtually odorless. The commercial material has a faint, pleasant-resinous odor.

Abietic acid is slightly bitter at concentrations of more than 50 ppm.

The acid is briefly mentioned in this work because of its close relationship – in chemical structure – to many Ambregris materials.

It is also the natural source and parent of several solvent-fixatives, used in perfumery: Abitol, Methyl abietate (Abalyn) and hydrogenated Methyl abietate (Hercolyn).

Rosin, the natural material, is occasionally used as a fixative in Pine and other fragrance types. It is inexpensive and has at times been popular in certain types of soap perfume.

Certain derivatives of Abietic acid are used as emulsifiers and "cloudificators" in carbonated beverages – to give visual impression of fruit juice content in beverages made with little or no "cloudy" natural juice. "Cloudy" Orange sodas are popular in certain countries.

Prod.: by distillation of Rosin (from American Turpentine, e. g.) or by treatment with acid to isomerize the natural Levopimaric acid. Purification over the Diamylammonium salt.

1-721; 26-382; 67-698; 90-157; 100-1; 104-632; 124-255;

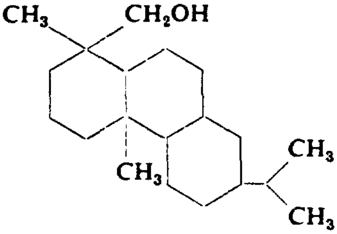
See also the following monographs:
Abitol,
Ambrein,
Dodecahydro tetramethyl furan,
Ethyl dodecahydro trimethyl furan,
Fixateur 404,
Manool,
Sclareol,
Squalene.

## 2: ABITOL

Hydroabietyl alcohol (technical grade).

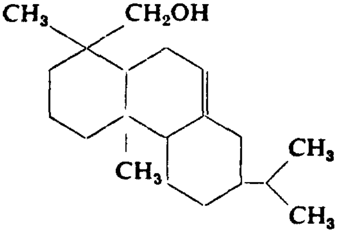
A primary monohydric alcohol consisting of approximately:

38 % Tetrahydro abietyl alcohol (1)
34 % Dihydro abietyl alcohol (2)
13 % Dehydro abietyl alcohol (3)
15 % Non-alcoholic components.



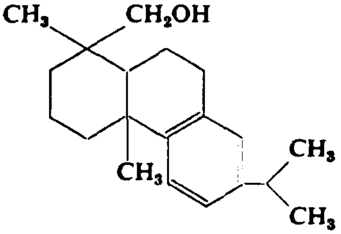
(1)

$C_{20}H_{36}O = 292.51$



(2)

$C_{20}H_{34}O = 290.49$



(3)

$C_{20}H_{30}O = 286.46$

Colorless tacky-viscous liquid, non-pourable room temperature. Sp.Gr. = 1.01.

Insoluble in water, miscible with alcohol, terpenes, essential oils and most perfume chemicals.

Very faint, woody and slightly piney odor. Intermittent heating may cause an increase in the odor level.

Excellent fixative for low-cost fragrances of pine, wood, fougère, new-mown-hay and other types. For industrial fragrances, household and soap perfumes, etc.

Produced from hydrogenated rosin acids.

67-717;
(Hercules Powder Co. Sept. 1965).
See also: Manool.
Sclareol.

## 3: ACETALDEHYDE

Ethanal.
Acetic aldehyde.
"Ethyl aldehyde".

$CH_3$—CHO

$C_2H_4O = 44.05$

Gas or colorless mobile liquid, boiling at°.8 C. Sp.Gr. 0.80.

Highly flammable. Vapors form explosive mixtures with air.

Sol. in water, alcohol and essential oils.

Pungent ethereal-nauseating odor, in high dilution reminiscent of Coffee or Wine.

Polymerizes easily to form Methaldehyde or Paraldehyde.

Used in minute amounts in artificial essential oils, occasionally as part of a topnote in perfumes.

In Flavors for: Apple, Apricot, Banana, Berry, Black Walnut, Butter, Chocolate, Coffee, Grape, Peach, Rum, Wine, etc. Concentration: 4–25 ppm in finished product.

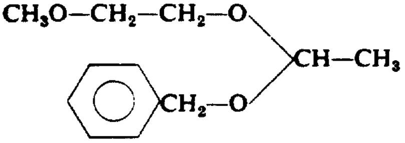
G.R.A.S. F.E.M.A. No.2003.

Produced from Ethyl alcohol, or Acetic acid, or Ethane, or Acetylene.

100–4; 30–245/247/248; 31–61; 89–9; 140–157; 159–411; 159–535;

## 4: ACETALDEHYDE-BENZYL-beta-METHOXYETHYL ACETAL

Benzyl methoxyethyl acetal.
*1*-Benzyloxy-*1*-(*beta*-methoxy)-Ethoxyethane.



$C_{12}H_{18}O_3 = 210,28$

Colorless liquid.
Mild, sweet, slightly green-fruity odor.

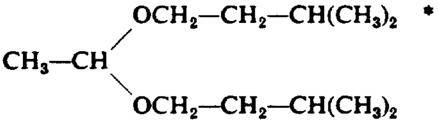
Used in minute traces in Cherry and other fruit flavors.

Rare material, usually manufactured by user, not offered commercially.

G.R.A.S. F.E.M.A. No.2148.

## 5: ACETALDEHYDE-DI-iso-AMYLACETAL

Ethylidene di-*iso*-amylether.
Di-*iso*-amylacetal.



$$CH_3-CH\begin{array}{l}\diagup OCH_2-CH_2-CH(CH_3)_2 \quad * \\ \diagdown OCH_2-CH_2-CH(CH_3)_2\end{array}$$

$C_{12}H_{26}O_2 = 202,34$

Colorless liquid. Sol. in alcohol and ess.oils.
Mild, oily-green, somewhat vegetable odor.

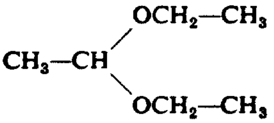
*Prod. from Acetaldehyde and Fusel-Amylalcohol or synthetic Pentanol. Consists therefore of a mixture of Pentanol-isomers.

Occasionally used in Coffee, Grape, Wine or fruit flavor compositions.

31-64; 31-65;

## 6: ACETALDEHYDE DIETHYLACETAL

Acetal.
Diethyl acetal.
Ethylidene diethylether.
*1,1*-Diethoxy ethane.



$$CH_3-CH\begin{array}{l}\diagup OCH_2-CH_3 \\ \diagdown OCH_2-CH_3\end{array}$$

$C_6H_{14}O_2 = 118,18$

Colorless liquid. Sp.Gr. 0.83. BP. 103° C.
Sol. in water: 5,5%.

Miscible with alcohol in all proportions.

Agreeable, refreshing, fruity-green odor.

Used in Apple, Apricot, Banana, Peach, Whisky and Wine flavors.

Concentration: 6–50 ppm in finished product.

In perfumery: topnote for Jasmin and other florals.

G.R.A.S. . F.E.M.A. No.2002.

Prod.:

1) from Acetaldehyde and alcohol with dehydrating agent or catalyst.
2) from Vinylacetate plus Ethanol with Boron trifluoride catalyst.

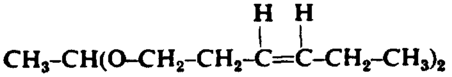
May polymerize on storage. Unstable under acid conditions (flavors!).

Fairly stable in alkali.

31-72; 66-483; 100-4; 140-157;

## 7: ACETALDEHYDE-DI-cis-3-HEXENYL-ACETAL

"Leaf alcohol acetal".



$CH_3-CH(O-CH_2-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_3)_2$

$C_{14}H_{26}O_2 = 226.36$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful, oily-green odor with a sweet, vegetable-like undertone. The greenness is not nearly as sharp or harsh as it is in the alcohol itself, and the overall effect of the acetal is also much weaker as compared to *cis-3*-Hexenol.

The use of this acetal has been suggested since the acetal is more stable in mild alkali, therefore of practical use in soaps, etc. The acetal is also an interesting item as a topnote ingredient in modern perfumes, as a modifier for Galbanum/Styrallylester complexes, in Oakmoss bases, etc.

It is unstable under acid conditions, and therefore not recommended for flavors in which acid is used.

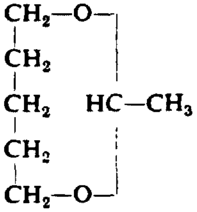
Prod.:

1) from Acetaldehyde and *cis-3*-Hexenol.
2) from Vinyl-*cis-3*-hexenyl ether and *cis-3*-Hexenol.

(sample: Compagnie Parento, Inc.)

## 8: ACETALDEHYDE-DI-PENTANEDIOL ACETAL

Acetaldehyde-pentamethyleneglycol acetal.
Acetaldehyde-*1,5*-dihydroxypentane acetal.



$C_7H_{14}O_2 = 130.19$

Colorless, slightly oily liquid. Soluble in alcohol and ess. oils.

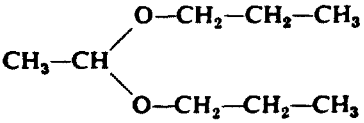
Poorly soluble in terpenes.

Mild, somewhat sweet-floral odor. Useful in artificial flower fragrances.

Prod.: from Pentamethylene glycol by condensation with Acetaldehyde.

## 9: ACETALDEHYDE-DI-n-PROPYL-ACETAL

Dipropyl acetal.
*n*-Propyl acetal.
Ethylidene dipropylether.



$C_8H_{18}O_2 = 146.23$

Colorless liquid. Soluble in alcohol and ess. oils.

Strong, ethereal-winey odor.

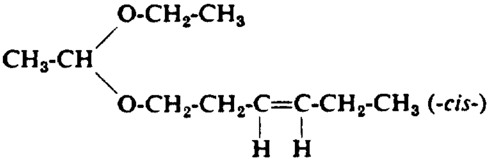
Use: sparingly in perfumes as a natural topnote, but it is less interesting than Acetal R. Trace amounts in fruit flavors: Pear, peach, etc.

Prod.: from Acetaldehyde and *n*-Propyl alcohol.

31-72;

## 10: ACETALDEHYDE-ETHYL-trans-3-HEXENYL ACETAL

"Leaf acetal".
A mixed acetal of Ethanol and "Leaf alcohol" with acetaldehyde.
Commercial products usually contain some *trans-4*-isomer.



$C_{10}H_{20}O_2$ = 172,27

Colorless mobile liquid. Miscible with alcohol and essential oils.

Powerful green, herbaceous-vegetable, oily odor, reminiscent of many natural products.

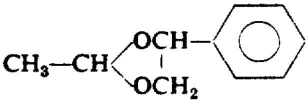
Used sparingly in floral perfumes to introduce a natural-green topnote, and in general as a topnote in mossy or citrusy perfumes.

Fairly stable in alkali, unstable in acid of $p_H$ lower than 5.

Prod.: from Acetaldehyde diethylacetal (Acetal) with cis-3-Hexenol.

## 11: ACETALDEHYDE-PHENYLETHYLENEGLYCOL ACETAL

Phenyl glycol acetal.
Acetaldehyde-*1*-phenyl-*1,2*-ethanediol acetal.
Styrene glycol acetal.
*2*-Methyl-*4*-phenyl-*1,3*-dioxolane.



$C_{10}H_{12}O_2$ = 164,21

Colorless oily liquid.

Sol. in alcohol and ess. oils.

Pleasant, but weak floral odor, suggestive of Rose and Jasmin, with undertones of green-earthy, herbaceous character.

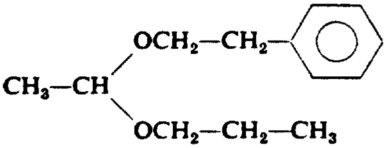
Useful in floral perfumes, including Jasmin, Gardenia, Tuberose, Rose, etc.

Prod.: from Acetaldehyde and Phenylethylene glycol.

31-72;

## 12: ACETALDEHYDE PHENYLETHYL-n-PROPYLACETAL

Acetal R (Givaudan).
Pepital.
A "mixed" acetal:



$C_{13}H_{20}O_2$ = 208.30

Colorless liquid. Miscible with alcohol and ess. oils.

Powerful, ethereal, green-herbal and leafy odor and very natural character.

Useful in perfumes as a topnote in moss-types, single florals and herbaceous chypres. Usually much less than 1 % in the perfume oil.

In flavors: traces in fruit flavors to introduce a green-winey note and greater naturalness.

Concentration: about 2-3 ppm. in the finished product.

Prod.: from Acetaldehyde-dipropylacetal and Phenylethyl alcohol.

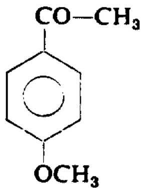
G.R.A.S. F.E.M.A. No.2004.

106-15;

## 13: ACETANISOLE

*para*-Methoxy acetophenone.
Anisyl methyl ketone (confusing name).
Methyl-(*4*-Methoxyphenyl)-ketone. (commercial grades of this chemical are mixtures of *para*- and *meta*-).

Heliopon.
Aubepinol.
Aubepinone.
Helional.
Melitone.
Epenone.
Estenone.
Crataegon.
*para*-Acetyl anisole.
Novatone.
Fernon.
Melilot.
Ketobepin (Mühlethaler).
Nyobepine.



(mainly *para*-)

$C_9H_{10}O_2 = 150.17$

Colorless crystals or fused crystalline mass. M.P. 36-38° C.

Heavier than water, practically insoluble in water. Miscible with oils, soluble in alcohol.

Sweet, but somewhat harsh, haylike odor with floral-animal notes. Suggestive of Hawthorne, Mimosa, Heliotrope, etc.

Relatively stable in soap and under similar, mild-alkaline conditions.

Used in woody-floral fragrances such as Cassie, Mimosa, Fougère, Chypre, New-MownHay, in herbaceous citrus types, etc.

In flavors for Butter, Caramel, Chocolate, Fruit, Nut, Vanilla, etc. Also in Tobacco flavoring, "tobacco sauce", etc.

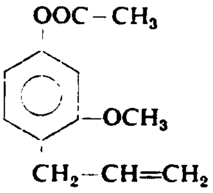
G.R.A.S. F.E.M.A. No.2005.

Prod. from Anisole plus Acetyl chloride.

4-86; 5-160; 7-268; 7-318; 41-13; 44-679; 103-270; 106-16; B-VII-87; 140-166;

## 14: ACETEUGENOL

Eugenol acetate.
Eugenyl acetate.
Acetyl eugenol.
Acetoeugenol.
Allyl guaiacol acetate.
*4*-Allyl-*2*-methoxyphenyl acetate.
*2*-Methoxy-*4*-allyl-*1*-phenylacetate.
*3*-Methoxy-*4*-acetoxy-*1*-allylbenzol.



$C_{12}H_{14}O_3 = 206.24$

White granular crystals, melting at 29° C. B.P. 282° C. The pale yellowish liquid material may remain supercooled as a liquid at room temperature. Sp.Gr. 1.08. Insoluble in water, soluble in alcohol and ess. oils.

Mild and sweet-spicy, balsamic-fruity odor, reminiscent of carnation. Earthy-fresh notes, or leafy-floral notes not uncommon.

Used in perfumes to emphasize floralness in carnation, along with *iso*-Eugenol, Amyl oxy-*iso*-eugenol, etc. Fresher than these, but also milder. Not stable in white soap or alkali.

In flavors for berry, fruit, mint, spice and vanilla types.

Concentration in candy: 0.5 to 20 ppm.

In chewing gum: up to 100 ppm. (in finished products).

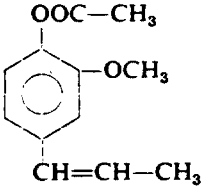
G.R.A.S. F.E.M.A. No.2469.

Produced from Eugenol by Acetylization.

43-504; 106-158; 140-170; 90-572;

## 15: ACET-iso-EUGENOL

*iso*-Eugenol acetate.
Acetyl-*iso*-eugenol.
Methoxy-*4*-acetoxypropenyl benzene.
*2*-Methoxy-*4*-propenyl phenylacetate.



$C_{12}H_{14}O_3 = 206.24$

White granular crystals. M.P. 80° C.

Insoluble in water, soluble 4% in Ethylalcohol, miscible with ess. oils. Sp.Gr. 1.087.

Fruity-balsamic, warm and faintly spicy odor, somewhat clove-like, but with rosy floral notes and vanilla-like sweetness.

Useful in floral perfume compositions, as a sweetener in herbaceous fragrances, and as a fixative in carnation perfumes.

May cause discoloration in white soaps.

In flavors for berry, fruit and spice compositions.

Concentrations from 0.4 to 17 ppm. in finished products.

Up to 100 ppm in chewing gums.

G.R.A.S. F.E.M.A. No.2470.

Produced from *iso*-eugenol by acetylization.

106-207; 140-171;

## 16: ACETIC ACID

Ethanoic acid.

$CH_3—COOH$

$C_2H_4O_2 = 60.05$

Colorless mobile liquid, congealing in the cold, melts at 16° C. Miscible with water, glycerin, alcohol, propylene glycol and (glacial acetic acid) with many essential oils of low hydrocarbon content.

Pungent, stinging sour odor, unpleasant when concentrated, less repulsive when diluted below 15% in water.

Clean-sour, acid taste, perceptible well below 1% in water.

Useful in flavor compositions: butter, butterscotch, cheese, chocolate, grape, raspberry, rum, spice, strawberry, vinegar, wine, etc.

Highest concentration in food (condiments) 6000 ppm (or one part in 170). However, concentrations up to 40,000 ppm (4%) in pickle brine have been observed.

G.R.A.S. F.E.M.A. No.2006.

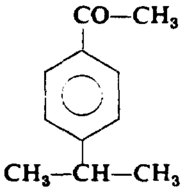
Prod.:

1) as a by-product in the dry distillation of wood (tar production).
2) from Acetylene via Acetaldehyde, by oxidation with air.
3) from Ethyl alcohol vapours over heated catalyst, then oxidized.
4) by biological activity: mainly in the vinegar production.

66-568; 100-6; 140-133; 158-157;

## 17: ACETOCUMENE

*para-iso*-Propyl acetophenone (commercial grade has considerable amounts of *meta*-isomer)
"Cumyl methyl ketone".
*para-iso*-Propyl acetyl benzol.
*para*-Acetyl cumol.
Methyl-(*4-iso*-Propyl phenyl) ketone.
*para*-Acetyl cumene.
*1,4*-Acetyl-*iso*-Propyl benzol.



$C_{11}H_{14}O = 162.23$

Colorless liquid. B.P. 252° C. Insoluble in water, soluble in alcohol, miscible with ess. oils.

Powerful, dry-herbaceous, woody-orrisy odor, remotely reminiscent of cuminic derivatives.

Rarely used in perfumery. Occasionally in Cassie and Mimosa bases.

Used in fruit and honey flavors, and in pickle flavoring.

Concentrations from 0.08 to 5 ppm in finished product.

G.R.A.S. F.E.M.A. No.2927.

Produced from Cumene + Acetyl chloride + $AlCl_3$ or directly from Benzol + Acetyl chloride + *iso*-Propylchloride (Friedel-Crafts Synth.).

5-162; 7-222; 31-83; 126-224;

## 18: ACETONE

Dimethyl ketone.
Propanone.
Ketopropane.

$CH_3—CO—CH_3$

$C_3H_6O = 58.08$

Colorless mobile liquid. B.P. 56° C.
Sp.Gr. 0.80.

Miscible with water, ethylalcohol, ether and most essential oils and perfume chemicals.

Flammable. Vapors form explosive mixtures with air.

Flash point −17° C.

Light ethereal-nauseating and powerful odor of very poor tenacity. Irritant at high concentration, rather pleasant in dilution.

Sweet and slightly burning taste.

Used as an extraction solvent for perfume and flavor materials, but rarely, if ever, as such in flavors. However, it forms an interesting part of the volatile portion of Coffee flavor and other food flavors. Occasionally used as a diffusive topnote in perfumes, or as an additive to colognes or other perfume solutions in order to make them smell more "ethereal"- aged, mellow.

Generally accepted tolerance – Acetone derived from Oleoresins: 30 ppm.

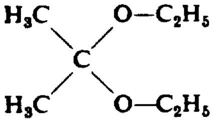
Produced synthetically from butanol, or from *iso*-propanol, or by biochemical synthesis from sugars or starches (fermentation process).

Also used in the synthesis of Ionones.

100-7; 1-176; 30-189; 30-250; 30-347; 31-109; 65-373; 66-514; 159-413; 162-567

## 19: ACETONE DIETHYLKETAL

Diethylal acetone.
Acetone diethyl acetal.



$C_7H_{16}O_2 = 132.19$

Colorless liquid. B.P. 114° C.

Soluble in alcohol, miscible with ess. oils and perfume chemicals.

Ethereal-camphorlike odor.

Stable when pure and at room temp.

Decomposes during heating in presence of moisture or traces of mineral acid.

Probably not used in flavors.

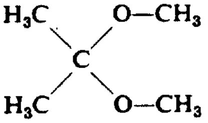
Occasionally used in perfumes to introduce diffusive topnotes in herbaceous-camphoraceous blends (Lavandin-Rosemary, etc.).

Produced by synthesis via orthoformic ester, or via vinyl ether, or via formiminoethylether hydrochloride.

31-115; 66-520;

## 20: ACETONE DIMETHYLKETAL

Dimethylal acetone.
Acetone dimethyl acetal.



$C_5H_{12}O_2 = 104.15$

Colorless liquid. B.P. 83° C.

Soluble in alcohol, miscible with ess. oils and perfume chemicals.

Ethereal odor.

Stable when pure and at room temp.

Decomposes into Acetone and Methanol during heating in presence of moisture or traces of mineral acid.

Presumably not used in flavors.

Rarely used in perfumes – for ethereal topnotes and "alcohol-like" effects.

Produced synthetically via orthoformic ester or vinyl ether. Also from formiminomethylether hydrochloride.

31-114; 66-520;

## 21: ACETONITRILE

Methyl cyanide.
Acetid acid, nitrile.

$CH_3—CN$

$C_2H_3N = 41.05$

Colorless liquid. B.P. 81-82° C. Sp.Gr. 0,78

Miscible with water. Insoluble in aqueous salt solution. Soluble in alcohol and ess. oils, perfume chemicals, etc.

Agreeable odor, mild and reminiscent of Bitter Almond oil, but less pronounced than Butyronitrile.

Not recommended for flavors, although toxicity is much lower than that of hydrocyanic acid.

Could be used in perfumes, but is probably too unstable in presence of moisture.

1-189; 30-261; 31-191; 66-601; 66-606;

## 22: ACETONYL ACETONE

2,5-Hexanedione.
*alpha-beta*-Diacetyl ethane.

$CH_3-CO-CH_2-CH_2-CO-CH_3$

$C_6H_{10}O_2 = 114.14$

Colorless liquid. B.P. 188° C. Sp.Gr. 0.974

Miscible with water, ethylalcohol and ether, ess. oils and perfume materials.

Pleasant, sweet-ethereal odor.

Possible use in perfumery for fresh-ethereal, winey topnotes. Presumably not used in flavors. Vapors are modestly toxic. Polymerizes on standing, turns yellowish and loses odor gradually.

Produced by hydrolysis of 2,5-dimethylfuran.

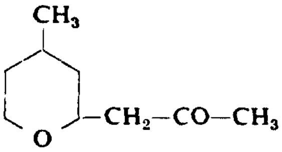
Also formed in Nature in the pyrolysis of Acetone. This has interest to the study of the synthesis of Rose Oxide and related chemicals. Another synthesis uses Sodium ethyl acetoacetate plus Iodine. This reaction is followed by decarboxylation by heating.

Acetonylacetone yields 2,5-Dimethylfuran by dehydration.

31-82; 66-724; 66-725; 100-8;

## 23: cis-ACETONYL-2-METHYL-4-TETRAHYDROPYRAN

A chemical related to Rose Oxide (see monograph).



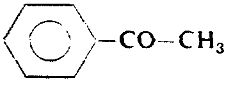
$C_9H_{16}O_2 = 156.21$

Colorless liquid of powerful, warm-spicy odor, reminiscent of breadcrust, burnt caramel, etc. with a fruity-floral, sweet note in extreme dilution.

Identified in Geranium oil (Y.-R. Naves 1963).

## 24: ACETOPHENONE

Phenyl methyl ketone.
Acetyl benzene.
Acetyl benzol.
Benzoyl methide.
"Hypnone".
Methyl phenyl ketone.



$C_8H_8O = 120.15$

Colorless liquid, solidifies in the cold. MP = 20°.5 C.

Slightly soluble in water, miscible with ethyl alcohol, essential oils and perfume chemicals. Sp.Gr. = 1.033.

Pungent-sweet odor, in dilution resembling that of hawthorn or a harsh orange-blossom type. The effect in perfumes is generally a flowery one, coumarin-like, warm, slightly animal, powerful. Concentration in perfume oils usually less than 1%. Mostly in low-cost fragrances, particularly for soap, detergents, industrial purposes, etc. Used in trace amounts in flavors for Almond, Cherry, Florals, Fruit, Strawberry, Tea, Tobacco, Tonka, Vanilla, Walnut, etc.

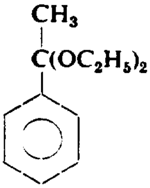
G.R.A.S. (1965-list). However, the author of this work suggests that caution be taken when using Acetophenone in food flavors. Acetophenone is a soporific, although its toxicity is lower than that of Coumarin, when using the $LD_{50}$ as a measure.
F.E.M.A. No.2009.

Acetophenone works well in perfume combinations with Anisaldehyde, Labdanum, Terpineol, Phenylacetaldehyde, etc.

156-1; B-VII-271; 106-23; 41-19; 44-679; 44-806; 65-474; 68-534; 5-157; 7-6; 1-520; 31-82; 140-166;

## 25: ACETOPHENONE DIETHYL KETAL

Acetophenone diethyl acetal.



$C_{12}H_{18}O_2 = 194.28$

Colorless liquid. Decomposes when heated near boiling point (approx. 215° C).

Warm, green-spicy, somewhat floral odor, varying according to the chemical purity of the product.

This material could find some use in perfume compositions as a modifier for Anisaldehyde and Acetanisole in New Mown Hay and various herbaceous fragrance types.

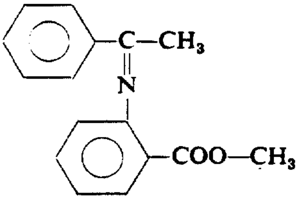
Prod. from Acetophenone and Ethyl orthoformate in Ethyl alcohol with hydrochloric acid.

Very rarely offered as a perfume chemical by commercial suppliers.

68-535;

## 26: ACETOPHENONE-METHYLANTHRANILATE

A condensation product similar to a "Schiff's Base".
Main component:



$C_{16}H_{15}NO_2 = 253.30$

Yellowish oily liquid. Soluble in alcohol. Poorly soluble in hydrocarbons (Terpenes), miscible with most perfume materials.

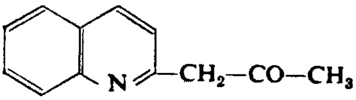
Heavy, sweet-floral, somewhat animal odor. The odor picture varies according to the quality of the reaction product. Preferred are the types in which the Acetophenone component is *not* the conspicuous note.

Very rarely used in perfumery, but often formed in compositions upon ageing of the perfume compound when it contains both chemicals, Acetophenone and Methyl anthranilate.

33-1029[2];

## 27: ACETOQUINALDINE

Acetyl-2-methylquinoline.



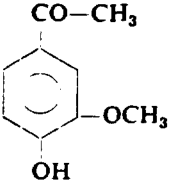
$C_{12}H_{11}NO = 185.23$

Although this material has been mentioned as being useful in industrial perfumery, the author would suggest that its hazard to human skin health and its general toxicity would decrease or possibly prevent its use in perfumes and flavors.

3-2; 4-2;
Deutsche Parfumerie Zeitung 1938, 293;

## 28: ACETOVANILLONE

Apocynin.
1-Hydroxy-*2*-methoxy acetophenone.
*3*-Methoxy-*4*-hydroxy acetophenone.
*1*-Hydroxy-*2*-methoxy-*4*-acetylbenzene.



$C_9H_{10}O_3 = 166.17$

White crystals or powder. M.P. 115° C.

Soluble in alcohol, essential oils and perfume chemicals. Slightly soluble in water at room temp. Easily soluble in hot water. Very faint, sweet odor, remotely reminiscent of Vanillin, but less spicy, somewhat fresher.

Occurs widely in Nature, including Orris root distillate.

Could find some use as a fixative in perfumery, but lends little odor to the compounds in which it is incorporated.

Not known to be used in flavors. Acetovanillone is a cardiac stimulant and a diuretic.

Prod. synthetically by methylation of *3,4*-Dihydroxy acetophenone. Also from Guaiacol acetate with Zinc chloride and Acetic anhydride. Can be isolated from the extract of the roots of Indian hemp, *Apocynum cannabinum L.*

Acetovanillone is an isomer of PAEONAL-see Methoxy hydroxy acetophenone.

1-523; 1-524; 12-45; 68-753; 100-94;

## 29: ACETYL ACETONE

*2,4*-Pentanedione.

$CH_3—CO—CH_2—CO—CH_3$

$C_5H_8O_2 = 100.12$

Colorless or very pale yellowish liquid.
B.P. 139° C. Sp.Gr. 0.97

Ethereal-minty odor, somewhat metallic or "chemical". In high dilution, the flavor in aqueous medium is sweet, remotely reminiscent of Peppermint sweetness.

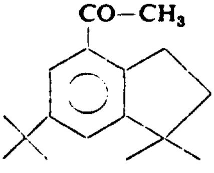
Not very stable. The enol form readily passes into equilibrium mixture.

Prod. from Acetone plus Ethyl acetate, or Acetone plus Acetic anhydride (with Boron trifluoride).

31-82; 66-723;

## 30: 4-ACETYL-6-tertiary-BUTYL-1,1-DIMETHYLINDAN

Celestolide (I.F.F.).
*4*-Acetyl-*1,1*-dimethyl-*6*-*tertiary*-butylindan.
An isomer of PHANTOLIDE – see Acetyl hexamethyl indane.



$C_{17}H_{24}O = 248.38$

Almost white crystals. Soluble in alcohol, miscible with essential oils and perfume chemicals.

Mild, sweet-musky odor with a faint, animal undertone and good tenacity. Relatively stable under normal conditions in perfume creations. May develop a slightly sour note during storage, a note which is appreciated by some perfumers, disliked by others.

Not known to be used in flavors.

Normal concentration in perfumes is 0.5 to 3%, but certain perfume types may benefit from considerably higher content of Celestolide.

Does not discolor soaps or other mildly alkaline products.

Prod. from *para*-Cymene.

156-284;

## 31: ACETYL-n-BUTYRYL

*2,3*-Hexanedione.
Methyl propyl diketone.

$CH_3—CO—CO(CH_2)_2CH_3$

$C_6H_{10}O_2 = 114.15$

Yellow oily liquid. B.P.128° C. Sp.Gr. 0.93

Slightly soluble in water, soluble in Propylene glycol, Ethyl alcohol and all common perfume and flavor materials.

Powerful, creamy-sweet, heavy-buttery, oily odor, yet somewhat milder than Diacetyl. Buttery-cheesy taste, particularly in acid medium. Odor is often classified as "quinone-like".

Rarely used in perfumery, perhaps in traces as a topnote in reconstituted essential oils, etc.

In flavors for its oily-"fermented fruit"-like taste and buttery notes.

Used quite frequently in Banana, Butter, Butterscotch, Cheese, Citrus, Pineapple, Rum, Strawberry, etc. imitation flavors.

Concentration in finished products:
5-8 ppm.

Prod. from Methyl butyl ketone or from Ethyl propyl ketone via the monoxime. Also from Acetoxy mesityloxide.

G.R.A.S. F.E.M.A. No.2558.

31-82; 66-721; 86-2; (Fritzsche Bros. Inc.);

## 32: ACETYL-iso-BUTYRYL

*4*-Methyl-*2,3*-pentanedione.
Methyl-*iso*-propyl diketone.

$CH_3—CO—CO—CH(CH_3)_2$

$C_6H_{10}O_2 = 114.15$

Yellow oily liquid. B.P. 116° C.
Sp.Gr. 0.921

Slightly soluble in water, soluble in Propylene glycol, Ethyl alcohol and all common perfume and flavor materials.

Heavy creamy-sweet, fruity-buttery odor, often described as "quinone-like". Less buttery, more fruity than the normal ketone (see previous monograph). Overall milder and weaker than Diacetyl.

Rarely, if ever, used in perfumery.

Frequently used in flavors for Banana, Butter, Butterscotch, Nut, Rum, Strawberry, etc.

Concentration in finished goods: usually 1-10 ppm.

G.R.A.S. F.E.M.A. No.2730.

Prod.: from Methyl-*iso*-butylketone.

86-2;

## 33: ACETYL CAPROYL

*2,3*-Octane dione.

$CH_3—CO—CO—(CH_2)_4—CH_3$

$C_8H_{14}O_2 = 142.20$

Yellowish oily liquid. B.P. 175° C.
Sp.Gr. 0.88.

Slightly soluble in water, soluble in alcohol and oils, in Propylene glycol and Glycerin.

Powerful and sweet, oily-buttery odor with herbaceous-cheesy undertone, yet not rancid or unpleasant in dilution.

Creamy-cheesy, mildly buttery taste in dilutions near 10 ppm.

The title Diketone is used on a very limited scale in perfume compositions, mainly as a trace component in topnote compositions, where it gives interesting effects in the presence of Civet and Phenylacetic acid, or certain Labdanum products, etc. It is also of good use in Ylang Ylang compositions and in many other flower bases.

The author has no record of its use in flavors.

Prod.:

1) from Ethyl Amyl ketone with Selenium oxide.
2) from Amylacetoacetate via its oxime.

4-41; 26-388; 66-721; B-I-795;

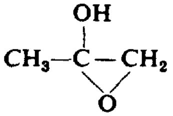
## 34: ACETYL CARBINOL

Acetol.
Hydroxy acetone.
Pyruvic alcohol.

$CH_3—CO—CH_2OH$

$C_3H_6O_2 = 74.08$

Exists partly in the tautomeric form:



Colorless liquid, miscible with water, alcohol, essential oils and perfume and flavor chemicals.

B.P. 146° C. Sp.Gr. 1.0824

Pungent, sweet-caramellic, somewhat choking-ethereal odor. Sweet, slightly burning taste.

The author knows of no use for this material in perfumery. Acetyl carbinol is used in flavor creation for Coffee, Caramel, Rum, etc. and the chemical has been identified in the vapors above steamed Coffee.

Polymerizes on standing, unless properly stabilized. May form a dimeric acetol ether.

Prod. from Bromoacetone plus sodium formate, followed by Methanol hydrolysis of the formed ester.

Or by biochemical synthesis from Propylene glycol with sorbose bacterium.

1-259; 46-231; 66-709;

## 35: ACETYL CARBINYL ACETATE

Acetol acetate.
Pyruvic acetate.

$CH_3—CO—CH_2—OOC—CH_3$

$C_5H_8O_3 = 116.12$

Colorless liquid, boiling at approximately 180° C.

Soluble in alcohol, Propylene glycol, essential oils, perfume and flavor chemicals.

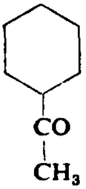
Peculiar fruity-buttery, somewhat sour odor. Butter-vinegar-like taste.

Could find use in flavors for Butter, Butterscotch, Rum, Nut, Cream, Cheese, etc.

47-296; also info. from F.Ritter & Co., Los Angeles, Calif., U.S.A.

## 36: ACETYL CYCLOHEXANE

Hexahydro acetophenone.
Methyl Cyclohexyl ketone.
Cyclohexyl methyl ketone.



$C_8H_{14}O = 126.20$

Colorless liquid, soluble in alcohol, essential oils and perfume materials.

Peculiar camphoraceous-sweet odor with a certain amount of floral tones.

Although this chemical would primarily lend itself to perfume compositions in the Pine, Wood, Herbaceous and other non-floral types, it has a similarity to the harsh-floral types such as Hyacinth, etc. and its sweetness is sometimes classified as "musky".

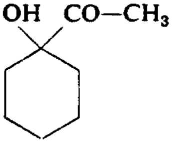
Rarely used in perfumes, probably never in flavors.

Prod. synth. from Cyclohexene via Acetyl cyclohexene, hydrogenated to Acetyl cyclohexane.

3-171; 67-215; 67-216;

## 37: ACETYL CYCLOHEXANOL

*1*-Acetylcyclohexan-*1*-ol.
*1*-Hydroxy-cyclohexyl methyl ketone.
Methyl-(*1*-oxy-cyclohexyl)ketone.



$C_8H_{14}O_2 = 142.20$

Colorless liquid. Sp.Gr. 1.06, Insoluble in water, soluble in ethylalcohol and perfume materials.

Camphorareous, minty-herbaceous, also somewhat floral odor.

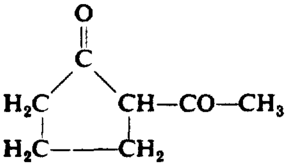
Poorer grades may show odor of Tetrahydro acetophenone (harsh-gassy odor).

Could find use in perfumery for its ability to "lift" and give diffusiveness ("radiation") to soap perfumes and lower-cost detergent perfumes, etc.

Prod. by hydration of 1-Ethynyl cyclohexanol.

B-VIII-505; 67-216;

## 38: 2-ACETYL CYCLOPENTAN-1-ONE



$C_7H_{10}O_2 = 126.16$

Colorless viscous liquid. Soluble in alcohol and perfume materials. Peculiar, warm-woody, somewhat herbaceous odor, reminiscent of Tobacco leaves (cured).

Useful in new perfume creations where non-floral notes may prevail, particularly along with Oakmoss products, Vetiver acetate, Indane musks, substituted coumarins, etc.

A few floral fragrance types may benefit from this chemical: Jasmin, Tuberose, Lily ("Bermuda Lily"), etc.

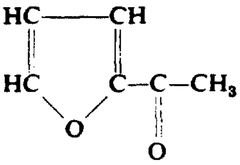
The author knows of no use of this chemical in flavors.

Prod. by intramolecular cyclization of Hexan-5-one-1-carboxylic acid.

67-110;

## 39: 2-ACETYL FURAN

Acetyl furan.
Methyl-*alpha*-furyl ketone.
*2'*-Oxo-*2*-ethyl furan.



$C_6H_6O_2 = 110.11$

Colorless crystals, turning yellowish when exposed to air and daylight. M.P. 30-32° C.

Soluble in Ethyl alcohol, essential oils, perfume and flavor chemicals and in Propylene glycol.

Powerful balsamic-sweet odor with a tobacco-like, almost narcotic pungency. Floral undertones are of balsamic-cinnamic character.

Could find use in reconstitution of essential oils and flower absolutes, or in traces as a powerful "lift"-ingredient in floral fragrances of the heavy, "exotic" type.

Not listed as G.R.A.S., probably not used in flavors anywhere.

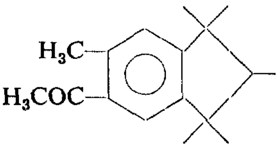
Produced as an isolate from Beech and Oak wood tar oils.

Fractions near the Acetyl furan fractions contain chemicals of Pyridine type, and may influence the odor quality of Acetyl furan made this way.

69-155;

## 40: 5-ACETYL-1,1,2,3,3,6-HEXAMETHYL INDAN

Phantolid (P.F.W.)



$C_{17}H_{24}O = 248.38$

Almost white crystalline mass melting at about 35° C to a viscous almost colorless liquid.

Soluble in Ethyl alcohol and perfume materials.

Sweet-musky, somewhat animal and slightly sour-sweaty odor of great tenacity. Blends excellently with Ionones, Sandalwood oil, and many non-floral, high-boiling perfume materials. Tends to develop a sour note during prolonged storage in closed containers.

Produces useful musky effects in perfumes at concentrations above 1%. Concentrations higher than 4-5% may cause perceptible misbalance in perfumes, unless the musk is accompanied by suitable blending materials of similar evaporation rate.

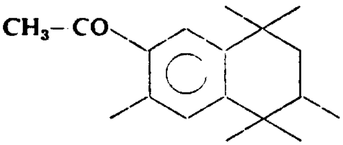
Produced from *para*-Cymene.

This material was one of the first low-cost "non-Nitro" musks offered to the perfume industry, and it opened new doors to the field of soap perfumery. Although no longer unique, and although many times outperformed by newer Indan-, Chroman-, macrocyclic and other non-Nitro musks at similar low cost, the title material deserves special mention for its pioneering position in the field of perfumery musks.

156-284; P.F.W. data steets;

## 41: 6-ACETYL-1,1,3,4,4,6-HEXAMETHYL TETRAHYDRONAPHTHALENE

"Tonalid" (Polak's Frutal Works).
(an isomer of Versalide).



$C_{18}H_{26}O = 258.41$

Colorless or white crystalline mass or fused, opaque mass.
M.P 46° C. B.P approx. 248° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet woody-musky odor of considerable tenacity. The degree of muskiness seems to vary with the concentration of the material in solution. At concentrations below 5 or 6% there is a marked improvement in the pleasant-musky notes, and very little, if any, hard-woody or unnatural chemical-musty notes. The latter may appear in higher concentrations, but odor descriptions vary significantly from one observer to another, and also with the age of the material.

This "Tetralin"-type musk was developed shortly after the first and temporarily successful "Phantolid" musk (see Acetyl hexamethyl indan) and the title material has been able to hold the market for quite some time in spite of violent competition from a wealth of new "Non-Nitro" musks, appearing on the perfume chemical market during the past decade.

The material has the advantage of good solubility in alcohol, no color or tendency of discoloration in functional products, but it does tend to produce "sour" notes in finished goods if the pH is slightly on the acid side (lower than 7).

The tenacity is distinctly inferior to that of Cyclopentadecanolide, and – in the author's opinion – also inferior to the Oxahexadecanolides.

But the material remains a remarkable milestone in the perfume chemistry and its use at present is mainly reduced by its relatively high cost in comparison to certain newer musks.

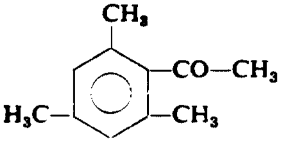
Many of the Indan- and Tetralin-type musks suffer from the fact that they appear as mixtures of several isomers and homologues as a result of the reaction by which they are manufactured.

Prod.: from *para*-Cymene and *tertiary*-Amylalcohol. Several methods are included in patents covering this basic method.

159-638; 159-639; 156-281;
see also: Versalide.

## 42: ACETYL MESITYLENE

Acetyl-*1,3,5*-trimethylbenzene.
*1,3,5*-Trimethyl acetophenone.
*2,4,6*-Trimethyl acetophenone.



$C_{11}H_{14}O = 162.23$

Colorless liquid, insoluble in water, soluble in alcohol and perfume materials. B.P 240.5° C
Sp.Gr. 0.9754

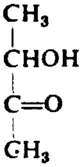
Peculiar, strong and persistent odor, simultaneously non-floral and heavy-sweet-floral. Not nearly as pungent as Acetophenone, but still rather chemical in its general character.

Could be used in perfumery as a modifier for basic components in New Mown Hay, Fougère, heavy florals, etc., and blends well with Labdanum, Nitromusks, Benzoates and Cinnamates, Coumarins, etc.

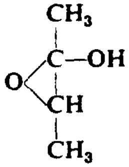
31-83; 68-532;

## 43: ACETYL METHYL CARBINOL

Acetoin.
Dimethyl ketol.
*2*-Butanol-*3*-one.
Methyl-*1*-hydroxyethyl ketone.
*3*-Hydroxy-*2*-butanone.
*gamma*-Hydroxy-*beta*-oxybutane.



or:



(Ketol form)

$C_4H_8O_2 = 88.10$

Pale yellowish liquid (depolymerized), or white microcryst. powder (polymer.) or white amorphous powder (polymer.).

There are two dimer forms: M.P. 85° C. and 95° C.

The liquid form solidifies in the cold and melts at 15° C.

Sp.Gr. 0.9972 (liquid form). 1.011 (dimer).

All forms are miscible with water, alcohol, Propylene glycol, Glycerine and common flavor materials. Poorly soluble in hydrocarbons. Dimer forms return to liquid monomer by simple solution, heat, distillation, etc.

Intensely creamy-fatty-buttery, penetrating odor, yet milder and less "quinone"-like than Diacetyl, not as sharp or volatile. Pleasant in extreme dilution.

Mild-creamy flavor in proper dilution, slightly sweet like mild cheese. Tends to decrease the power of other flavor ingredients, remove sharp or pungent notes, improve "body" and richness. Aqueous solutions of Acetoin are almost odorless. Flavor is perceptible at concentrations near 1 ppm, down to 0.2 ppm according to individual sensitivity. Used extensively in baked goods (up to 30 ppm), in Butter, Butterscotch, Caramel, Cheese, Coffee, Coconut, Creamsoda, Fruitflavors (Raspberry in particular), Strawberry, Nut, Rum, Vanilla, Walnut, and in many alcoholic beverages. Concentrations vary from 0.5 ppm to 30 ppm. and Acetoin is often accompanied by approximately one-tenth its amount of Diacetyl in such flavors.

G.R.A.S. F.E.M.A. No.2008.

Acetoin occurs naturally in bread, cheese, milk, butter, wine, fermented sugar, meats.

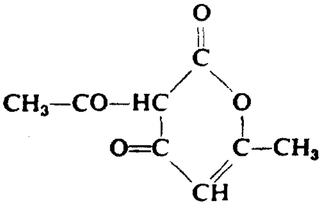
Produced from Diacetyl by partial reduction, or by oxidation of *2,3*-Butanediol with Sorbose bacterium or by bacterial fermentation of sugar, also by fungi (Aspergillus or Penicillium).

Acetoin may oxidize upon storage under poor conditions and form Diacetyl.

1-260; 3-2; 30-450; 100-7; 66-710; 157-185; 160-776;

## 44: 3-ACETYL-6-METHYL-2,4-PYRANDIONE

*3*-Acetyl-*6*-methyl-*1,2*-pyran-*2,4(3H)*-dione.
Methyl acetopyronone.
Dehydroacetic acid (a more common name in chemical literature).
"D.H.A."
*6*-Methyl-*3*-aceto-*2,4*-pyrandione.



$C_8H_8O_4 = 168.15$

White or colorless scaly crystals. M.P. 110° C. (under sublimation).

B.P. 270° C. Almost insoluble in water, soluble in most hydrocarbons, but only about 3% soluble in alcohol and about 1.5% in Propylene glycol. Being an acid, it is soluble in aqueous alkali under formation of alkali salt.

When pure and dry, almost odorless. Slightly bitter-sweet taste.

Although this material is not classified as a flavor chemical, it finds extensive use as a fungistat or fungicide at concentrations from 250 ppm or higher. It is common practice to use the water-soluble Sodium salt for easier introduction in products which are of acid Nature. The fungistat performs best under acid conditions. The Sodium salt has practically no odor and no taste in the dilution normally used.

It is interesting to note the similarity of this structure to the structure of Palatone (see monograph) and *iso*-Maltol (see that monograph). Both of these materials have some effect as fungistats.

The fungicidal and bactericidal effects of the title material are utilized in a great variety of consumer products, including toothpaste, where its anti-enzymatic effect is of value.

Prod.:
1) from Ethyl acetoacetate by self-condensation under mildly alkaline conditions (Sodium bicarbonate).
2) by polymerization of Ketene, obtained by thermal decomposition of Acetone).

26-472; 66-873; 100-322; B-XVII-559; 160-952;

## 45: ACETYL PROPIONYL

*2,3*-Pentanedione.
*beta-gamma*-Dioxopentane.

$CH_3—CO—CO—CH_2—CH_3$

$C_5H_8O_2 = 100.12$

Yellow liquid. B.P. 108° C. Sp.Gr. 0.9565.

Soluble 7% in water, miscible with alcohol and flavor materials, Propylene glycol and Glycerin.

Oily-buttery odor, pungent and somewhat "quinone"-like, less sharp and volatile than Diacetyl.

Aqueous solutions taste sweet, the oily-buttery aroma appears only at higher concentration where odor interferes with actual taste. Weak aqueous solutions are practically odorless.

Useful in flavors for Butter, Caramel, Cheese, Cream, Fruit, Rum, etc. at concentrations equal to 0.3 to 10 ppm in the finished consumer product. Little, if any, is used in perfumes.

Produced from Ethyl acetoacetate or from Diethyl ketone, or from Methyl propylketone.

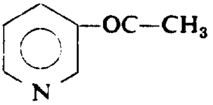
Not very stable on storage. May form a quinone by self-condensation.

G.R.A.S. F.E.M.A. No.2841.

B-I-776; 48-219; 66-721; 85-57; 86-3; Fritzsche Bros. info.

## 46: 3-ACETYL PYRIDINE

*beta*-Acetyl pyridine.
Methyl-*3*-pyridyl ketone.



$C_7H_7NO = 121.14$

Yellowish volatile liquid. Solidifies in the cold and melts at 14° C. B.P. 220° C.

Powerful, almost choking, Cigar-tobacco-type odor, which becomes pleasant only at extreme dilution, then also more typical tobacco-like.

Although Pyridine as such is G.R.A.S. (1965-list), there is no reference that 3-Acetyl pyridine is harmless, and proper caution should be exercised when this chemical is applied in perfumery. It is not reported as a flavor material.

However, at the concentrations needed for useful perfumery effect, there is little reason to believe that 3-Acetyl pyridine could ever become a hazard.

In certain types of flower bases, substitutes for flower absolutes, etc. this chemical can produce interesting and desirable effects. Lily, Jasmin, Tuberose, etc. are types of floral fragrances that may benefit from this effect.

Produced from Ethyl nicotinate and Ethyl acetoacetate, in principle by hydrolysis of Aceto acetylpyridine.

69-555;

## 47: ACETYL VALERYL

*2,3*-Heptanedione.
Valeryl acetyl.
Acetyl pentanoyl.

NOTE: Commercial products labelled ACETYL VALERYL are often actually ACETYL-*iso*-VALERYL (see next).

$CH_3CO—CO—(CH_2)_3CH_3$

$C_7H_{12}O_2 = 128.17$

Yellowish liquid, slightly soluble in water, miscible with alcohol, essential oils and flavor materials.

Powerful, diffusive, buttery and slightly animal, quinone-like odor, pungent and cheesy, but sweet in its oily character.

Aqueous solutions taste sweet, weak solutions are virtually odorless.

Useful in flavors for Butter, Cheese, Fruit, Nut, Rum, Raspberry, Strawberry, etc.

Concentrations vary from 1 to 10 ppm in the finished consumer product.

Acetyl valeryl may discolor in combinations containing Anthranilates, Indole, Quinolines, etc.

Produced from Butyl acetoacetate, or from Ethyl butyl ketone, or from Methyl-*n*-amylketone. (*2*-Heptanone).

G.R.A.S. F.E.M.A. No.2543.

Fritzsche Bros. info.
66-721;

## 48: ACETYL-iso-VALERYL

*5*-Methyl-*2,3*-hexanedione.
Acetyl-*iso*-pentanoyl.

NOTE: Commercial products sold under the name ACETYL VALERYL are often actually: ACETYL-*iso*-VALERYL.

$CH_3—CO—CO—CH_2—CH(CH_3)_2$

$C_7H_{12}O_2 = 128.17$

Yellowish liquid, slightly soluble in water, miscible with alcohol, Propylene glycol, Glycerin, essential oils and flavor materials.

Powerful oily-buttery, somewhat fruity odor (diff. from Acetyl Valeryl), quinone-like, rather pungent and mild animal, cheesy.

Aqueous solutions are almost odorless and taste sweet.

Used for purposes similar to those listed for Acetyl valeryl, however, the effect is more fruity than that of Acetyl valeryl.

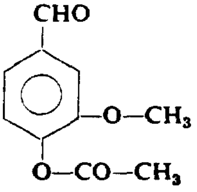
Prod. from Ethyl-*iso*-butyl ketone.

66-721;

## 49: ACETYL VANILLIN

This material is often called Vanillin acetate, but the author has preferred to use the title Acetylvanillin in view of the numerous possibilities of confusion in the nomenclature of acetylated Vanillins.

See below for monographs on related materials.



$C_{10}H_{10}O_4 = 194.19$

Colorless needle-like or plate-like crystals. M.P. 77° C.

Poorly soluble in water, soluble in alcohol and oils.

Mild and sweet, floral-Vanilla-like odor of good tenacity. Fresher than the odor of Vanillin, but lacks the warmth of Vanilla and Vanillin.

This material is used in spice flavor blends and in Vanilla flavor compositions as a modifier for Vanillin and related derivatives. It tends to reduce the overall power of the flavor, but also improve the total picture in "freshening-up" the heavy aroma of Vanillin, Ethylvanillin, etc.

The author finds that the title material is not used in perfume compositions to any large extent.

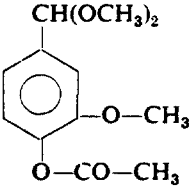
Prod.:
1) from Acetic anhydride plus an alkaline salt of Vanillin.
2) by oxidation of Acetyl-*iso*-eugenol.

G.R.A.S. F.E.M.A. No.3108.

72-151; 90-508;
See also the following monographs:
Acetovanillon.
Acetylvanillin dimethylacetal.
Vanillyl acetate.
Vanillylidene diacetate.
Vanillin triacetate.

## 50: ACETYLVANILLIN DIMETHYLACETAL

Vanillin acetate dimethylacetal.



$C_{12}H_{16}O_5 = 240.26$

The title material which is offered commercially from manufacturers of perfume chemicals, is briefly mentioned in this work in an attempt to elicidate the nomenclature of acetylated Vanillins, the names of which are often confused.

The intention behind the marketing of an acetal of Vanillin is clearly indicated: to offer a material of little or no skin-irritating effect as a substitute for Vanillin.

Modern literature claims that Vanillin does not form Acetals, and if this is correct, there is reason to believe that the title material is actually triacetate (see monograph), also called Acetylvanillin diacetate.

The latter material has very little odor and is of no substantial use to the perfumer. It is included in this work as part of the explanation supplied on the acetylated Vanillins.

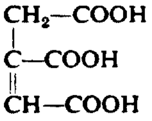
If, however, Acetylvanillin does form an Acetal, this monograph may serve as a basis for further elucidation of the small problem.

90-513: Acetals can not be formed.
156-350: Acetals have been prepared according to U.S. pat. No. 2,563,325 of 7th August 1951.

## 51: ACONITIC ACID

*1*-Propene-*1*,*2*,*3*-tricarboxylic acid.
Achilleic acid.
Citridic acid.
Equisetic acid.
*2*-Carboxy glutaconic acid.

Exists in *cis*- and *trans*-forms, the *trans*- being the more stable.



$$\begin{array}{l} CH_2\text{—}COOH \\ \,| \\ C\text{—}COOH \\ \,\| \\ CH\text{—}COOH \end{array}$$

$C_6H_6O_6 = 174.11$

M.P. (trans-) 194-195° C.

Colorless (white) crystal leaves or plates.

Soluble 16% in water at 13° C., 33% in water at 25° C. Decomposes when heated to 200° C.

Soluble in alcohol and most perfume and flavor materials, poorly soluble in hydrocarbons (Terpenes, etc.).

Practically odorless, but has pleasant winey-acid taste in aqueous solution.

Useful for Brandy, Fruit and Rum flavor. Concentrations may be as high as 30 ppm in the finished product.

Produced from sugar cane juice (molasses) or by dehydration of citric acid with sulfuric acid, or by catalytic dehydration. The *trans*-isomer is manufactured by above methods.

G.R.A.S. F.E.M.A. No.2010.

100-15; 66-1152; 1-290; 160-786;

## 52: ACROLEIN

Acraldehyde.
*2*-Propenal.
Acrylic aldehyde.
Acrylaldehyde.

$CH_2=CH-CHO$

$C_3H_4O = 56.06$

Colorless mobile liquid. Soluble about 30% in water, miscible with alcohol and oils.

Sp.Gr. 0.838 at 20° C., 0.862 at 0° C. B.P. 52°,5 C.

Resinifies easily in air unless stabilized (e.g. by small amount of a polyphenol). Daylight enhances polymerization and formation of a plastic solid, Disacryl.

Pungent, irritating odor (A. is a lachrymator), unbearable to human mucous membranes or eyes. The odor resembles that of an extinguished stearin candle (in the vapors of which A. is actually present). The odor is also classified as acrid.

Acrolein as such is rarely, if ever, used in perfumes or flavors, but it constitutes a very important intermediate material in Nature's and man's synthesis of many important perfume and flavor materials. Acrolein is therefore often present in these as a trace impurity.

Acrolein can be produced by dehydration of Glycerin with Potassium bisulfate, or in vapor phase by passing the glycerin vapors over Magnesium sulfate.

In spite of its repulsive odor and effect on human senses, Acrolein is not regarded as toxic, and its hazards are more that of being highly flammable than being poisonous.

1-168; 2-206; 31-36; 66-502; 100-17; 170-786;

## 53: ACRYLIC ACID

Propenoic acid.
Vinylformic acid.
Ethylene carboxylic acid.

$CH_2=CH-COOH$

$C_3H_4O_2 = 72.06$

Colorless liquid, solidifies in the cold, melts at 13° C.

Miscible with water, alcohol and most oils and perfume/flavor chemicals. Sp.Gr. 1.0621 B.P. 141° C.

Its odor resembles that of acetic acid, but it is more acrid, corrosive to human mucous membranes, irritating to the eyes. Polymerizes in air, unless properly stabilized. The polymers are mostly solid and odorless.

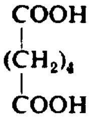
Rarely used in perfumery, occasionally used in flavor work. Esters of acrylic acid are used in certain industrial perfumes. Its toxicity can be classified as modest to low.

Produced by dehydration of Ethylene cyanhydrin, or Acetaldehydecyanhydrin, followed by hydration. Many other methods are used commercially, since Acrylic acid is an important chemical intermediate.

30-241; 30-242; 31-198; 66-630; 100-17; 160-788;

## 54: ADIPIC ACID

Hexanedioic acid.
*1,4*-Butane dicarboxylic acid.



$$\begin{array}{c}COOH\\|\\(CH_2)_4\\|\\COOH\end{array}$$

$C_6H_{10}O_4 = 146.14$

White (colorless) crystals or crystalline powder. M.P. 152-153° C.

Slightly soluble in water, about 1.4%. pH of that solution is 2.7 (25° C.). Soluble in ethyl alcohol, flavor materials, but very poorly soluble in Monoterpenes (Citrus oils, etc.).

Soluble about 60% in boiling water.

Practically odorless. Aqueous solutions have pleasant sour taste.

Used in fruit flavors as an acidifier, and in baking powder in place of Tartaric acid. Adipic acid is not hygroscopic and is therefore more suitable for baking powders. Acidifying strength approximately equal to that of Citric acid.

Concentration in finished product may be as high as 5.000 ppm (1 part per 200) in Gelatin desserts, etc.

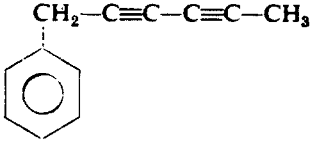
Prod. by oxidation of Cyclohexanol or Cyclohexanone.

G.R.A.S. F.E.M.A. No.2011.

66-981; 100-22; 77-189; 160-788; 140-147;

## 55: AGROPYRENE

*1*-Phenylhexa-*2,4*-diyne.
Capillen.



$C_{12}H_{10} = 154.20$

B.P. 140-143° C. Sp.Gr. 0.974.

Almost colorless or pale yellowish crystals, or pale yellowish liquid. Poorly soluble in alcohol, miscible with essential oils and most perfume chemicals.

Very unstable under UV-light or plain daylight. Oxidizes easily, and turns darker yellow.

Peculiar sweet-medicinal odor, reminiscent of Anise, Estragon, etc. with a herbaceous-minty note, quite tenacious.

Could find some use in perfumes and flavors, if it were made commercially available. Agropyrene constitutes more than 90% of the essential oil of Agropyrum repens (Couch-grass).

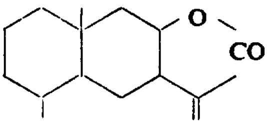
A. can be produced synthetically via the ketone Capillin made from Benzaldehyde plus Pentadiyne, followed by oxidation.

Also from Phenylacetaldehyde plus Methylethylketone followed by dehydration.

70-73; 87-414; 11-95; 65-16;

## 56: ALANTOLACTONE

"Helenin" (Mixture of two isomers and a Dihydro-derivative).
"Alant-camphor" (old name).



$C_{15}H_{20}O_2 = 232.31$

Soluble in alcohol and essential oils, perfume chemicals, etc. Colorless prismatic needle crystals. M.P. 78-79° C.

Peculiar sweet-minty, slightly woody odor, faint but tenacious.

Bitter taste, but not powerful.

Alantolactone constitutes almost 50% of the essential oil of Elecampane, accompanied by *iso*-Alantolactone and Dihydro alantolactone, possibly also Dihydro-*iso*-alantolactone.

Alantolactone can be isolated from this oil.

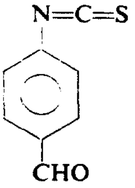
Although Alantolactone as such is not reported as used regularly in perfumes or flavors, it has medicinal value for many hundred years in the shape of extracts of the Elecampane root.

A number of Ambergris-smelling perfume chemicals have been prepared from Alantolactone.

7-164; 60-Febr.-34; 65-691; 90-639;

## 57: 4-ALDEHYDO-PHENYL THIOCARBIMIDE

"Thiotrope Base".
*para*-Thiocarbimide benzaldehyde.
*para*-Aldehydo phenyl-*iso*-thiocyanate.
*4*-Rhodan-benzaldehyde (Beilstein).



$C_8H_5NOS = 163.20$

White crystals or colorless needle-like crystals. Soluble in alcohol and oils.

Powerful, heavy-sweet, somewhat floral odor, resembling that of Heliotropine.

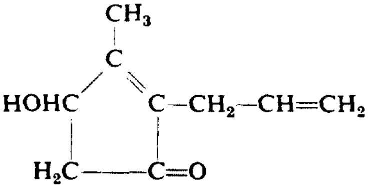
This material is generally considered obsolete in perfumery, having no special advantage over Heliotropine, and having poorer stability, more limited application than that aldehyde.

It is merely listed for its scientific and academic interest, and for the study of structure/odor relation.

7-396; 30-263; 31-38;

## 58: ALLETHROLONE

A commercial chemical, the chief component of which is:
*d,l-2*-Allyl-*4*-hydro-*3*-methyl-*2*-cyclopenten-*1*-one.



$C_9H_{12}O_2 = 152.20$

Yellowish or amber colored liquid.

Soluble in alcohol, miscible with essential oils and perfume chemicals.

Pungent, herbaceous-oily and heavy-sweet odor of considerable tenacity and displaying a gamut of "natural" odors.

NOTE: this material is considered toxic to human beings.

Produced as an intermediate in the manufacture of insecticides (Benzol Products, Inc.).

Although this material has been suggested as a useful perfume material in artificial flower absolutes, etc., it is generally considered too hazardous for any type of cosmetic product.

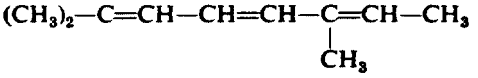
The material is mainly interesting because of its close chemical relationship to "Cyclotene" (Methylcyclopentenolone) and farther away, its relationship to the Jasmones.

It is also interesting to note the close relationship between Allethrolone, Pyrethrolone and the Jasmones, the two former having a Methyl chrystanthemumate included in their molecules.

100-31; (related matl.); 67-100 (related matls.);

## 59: ALLO-OCIMENE

*2,6*-Dimethyl-*1,5,7*-octatriene.
Commercial product is a mixture of stereoisomers.



$(CH_3)_2{-}C{=}CH{-}CH{=}CH{-}\underset{\displaystyle CH_3}{\underset{|}{C}}{=}CH{-}CH_3$

$C_{10}H_{16} = 136.24$

Sp.Gr. 0.82.

Colorless mobile liquid. Soluble in alcohol (when fresh and unpolymerized), poorly soluble when polymerized. Insoluble in water. Miscible with essential oils and perfume chemicals.

Polymerizes under exposure to air.

Diffusive, fresh-gassy, herbaceous odor. The gassy notes are more predominant in poorer grades of Allo-ocimene, almost imperceptible in good grade matl.

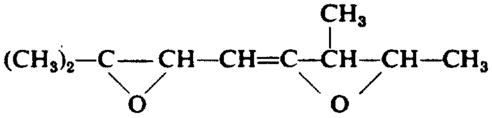
Useful in low-cost fragrances for industrial purposes, and in general as a lifting topnote, modifier for Limonene, etc. cheaper than Ocimene.

Produced by pyrolysis of *alpha*-Pinene in closed tube.

31-5; 100-740; 1-710;

## 60: ALLO-OCIMENE DIOXIDE

"A.O.D." (Newport Industries).
*1,6*-Dimethyl-*2,3*-and-*5,7*-bis-epoxy-*4*-octene.



$C_{10}H_{16}O_2 = 168.24$

Almost colorless or pale straw-colored liquid.

Sweet, woody-caramellic, rather mild odor of Furan-type, the woody notes resembling the odor of sawdust.

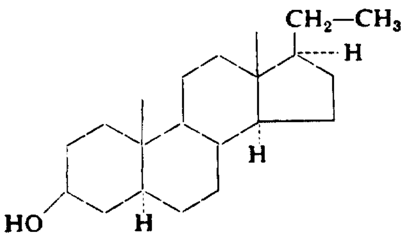
Bitter-sweet taste.

Could find use in perfumery in the reconstruction of essential oils and flower absolutes. At use levels of 1 to 3% it may introduce very "natural" woody-haylike, herbaceous-sweet topnotes. Also interesting as a component of low-cost industrial fragrances.

(Tenneco-Newport, N.Y. 1966 info.)

## 61: 3-alpha-ALLOPREGNANOL

A chemical belonging to the group of Gestogens (sex hormones).



White crystals. M.P. 182° C.

$C_{21}H_{36}O = 304.52$

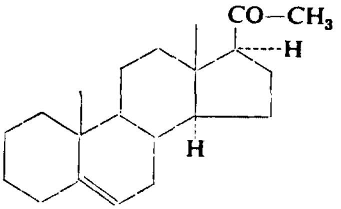
Musky odor of considerable tenacity, but low odor level. The odor becomes more perceptible when A. is incorporated in compositions with lower boiling perfume materials.

This chemical is not considered a perfume material, although it has been produced on a commercial scale by pharmaceutical research laboratories. To the author's knowlegde, it has not found use in marketed perfumes.

30-282; 67-908;
see further literature references under monograph: Androstenone.

## 62: 17,20-ALLOPREGNEN-3-ONE

A chemical belonging to
the group of Gestogens (sex hormones).



$C_{21}H_{32}O = 300.49$

White crystals. Soluble in alcohol and oils.

Very faint, but tenacious sweet-woody odor with some resemblance to Cedarwood. Trace of animal notes.

This chemical is listed merely for academic reasons as a representative of a very large group of chemicals, many of which have odors that could make these chemicals interesting for and applicable in perfumery.

Although most of these chemicals are commercially available, they are not produced for perfumery purposes, and their price level is generally prohibitive for their utilization in perfumery.

30-282; 67-903;
see further literature references under monograph: Androstenone.

## 63: ALLYL ACETATE

*2*-Propenyl acetate.
*1*-Propenyl-*3*-acetate.
Vinyl carbinyl acetate.
*2*-Propenyl ethanoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}CH_3$

$C_5H_8O_2 = 100.12$

Colorless mobile liquid. B.P. 98-100° C.
Sp.Gr. 0.928.

Insoluble in water, miscible with alcohol, essential oils, perfume and flavor chemicals.

Ethereal-winey odor, somewhat similar to that of Ethyl acetate, but more pungent, rum-like, fruity, arak-like.

Useful in flavors for Rum, Pineapple, Arak, Brandy, etc.

The taste at 50 ppm is sweet fruity-winey, ethereal, pleasant.

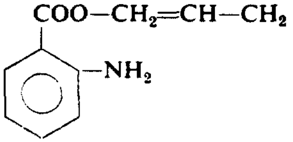
Allyl acetate is unstable in acid media if the $p_H$ is lower than 5.

Produced by azeotropic esterification of Allyl alcohol with Acetic acid.

31-123; 66-586; 86-4; B-II-136; 26-394; 160-770;

## 64: ALLYL ANTHRANILATE

Allyl-*ortho*-aminobenzoate.
*2*-Propenyl anthranilate.
Vinyl carbinyl anthranilate.



$C_{10}H_{11}NO_2 = 177.21$

Colorless or pale yellowish liquid.

Almost insoluble in water. Miscible with alcohol and oils, poorly soluble in Propylene glycol.

Sharp-fruity, very heavy balsamic-grapelike, sweet odor with a somewhat green topnote. The odor pattern varies according to the chemical quality of the material, and also to the method of production.

Useful in perfumes as a fixative for slightly green-citrusy fragrances, Petitgrain-Neroli types, etc. Relatively weak, but quite tenacious.

Traces are used in various fruit flavors, and particularly in Grape flavors (imitation grape).

G.R.A.S. F.E.M.A. No.2020.

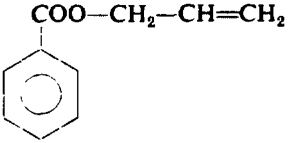
Produced by alcoholysis on Isatoic anhydride and Allyl alcohol, using Sodium methylate catalyst.

The cross-esterification method yields a very impure material.

47-296; 86-4; 77-213;

## 65: ALLYL BENZOATE

*2*-Propenyl benzoate.
Vinyl carbinyl benzoate.



$C_{10}H_{10}O_2 = 162.19$

Colorless liquid. (Yellowish if made by old cross-esterification method). B.P. 230° C. Sp.Gr. 1.058.

Insoluble in water, miscible with alcohol, perfume oils, flavor materials. Poorly soluble in Propylene glycol.

Weak, but pleasant berry-like, fruity odor with some cherry caracter (American type cherries).

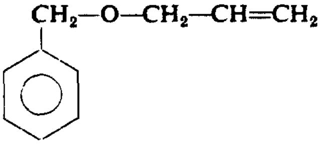
Useful in flavors, but must be free from Allyl alcohol. Rarely, if ever, used in perfumes.

Produced by direct esterification (azeotropic) of Allyl alcohol and Benzoic acid.

26-394; 47-296; 86-4;

## 66: ALLYL BENZYL ETHER

Benzyl allyl ether.
Benzyl allyl oxide.
Allyl benzyl oxide.
Propenyl benzylether.



$C_{10}H_{12}O = 148.21$

Colorless liquid. B.P. 205° C.

Sweet-ethereal odor with somewhat fruity undertone.

Could find use in perfumery, but the matetial as such is not very interesting or characteristic, does not offer any specific olfactory advantage.

Prod.: from Allyl bromide plus Sodium benzoylate.

## 67: ALLYL BUTYRATE

Propenyl butyrate.
Allyl-*n*-butyrate.
Vinyl carbinyl butyrate.

$CH_2{=}CH{-}CH_2{-}OOC{-}CH_2{-}CH_2{-}CH_3$

$C_7H_{12}O_2 = 128.17$

Colorless liquid. B.P. 143° C.

Insoluble in water. Miscible with alcohol and oils.

Fruity odor, somewhat Peach-Apricot-like, also resembling Apple.

Flavor in acidified aqueos sugar media: Apple-Apricot type.

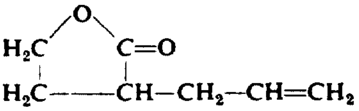
Useful in imitation fruit flavors: Apple, Apricot, Pineapple and – in traces – in Butter flavors.

G.R.A.S. F.E.M.A. No.2021.

Produced from Allyl alcohol and *n*-Butyric acid by direct esterification (azeotropic conditions).

26-394; 47-296; 77-185; 86-4; 140-139;

## 68: alpha-**ALLYL**-gamma-**BUTYROLACETONE**



$C_7H_{10}O_2 = 126.16$

Colorless or faintly yellowish oily liquid.
B.P. higher than 220° C. Sp.Gr. 1.0337.

Insoluble in water, miscible with alcohol and essential oils, poorly soluble in Propylene glycol.

Musky-herbaceous, heavy odor, reminiscent of Cumin, Angelica, Mintleaf.

The flavor is rather unpleasant, "perfumey" and unnatural.

This material could find use in perfumery as a modifier for Heptalactone and Octalactone, in combination with Coumarin for herbaceous notes, as a sweetener in Citrus fragrances, etc. However, its cost is still prohibitive and far too high for the actual odor value of this lactone.

Not reported as used in flavor work.

Produced from Allyl malonic ester and Ethylene oxide.

30-254; 31-170; 86-4;

## 69: ALLYL CAPRATE

Allyl caprinate.
Allyl decylate.
Allyl decanoate.
*2*-Propenyl decanoate.
Vinyl carbinyl decanoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_8{-}CH_3$

$C_{13}H_{24}O_2 = 212.34$

Colorless liquid. B.P.230° C. Sp.Gr. 0.89.

Insoluble in water, miscible with alcohol, essential oils and flavor chemicals.

Banana-Pineapple type odor, somewhat fatty-sweet and powerful without being pungent.

Very sweet, fruity taste, slightly fatty with an initial sharpness reminiscent of Pineapple notes.

Rarely used in perfumes.

Occasionally used in flavors as a modifier and volume-increasing fixative in Banana and Pineapple imitation. It blends well with Allyl caproate and Allyl caprylate, Ethyl decanoate, Ethyl heptoate, Nonanolide, etc.

Produced by direct esterification of Allyl alcohol with Decanoic acid, under azeotropic conditions (starter-catalyst).

35-851; 35-854;

## 70: ALLYL CAPROATE

Allyl hexanoate.
Allyl-*n*-hexoate.
*2*-Propenyl hexanoate.
Vinyl carbinyl hexanoate.
Allyl hexylate.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_4{-}CH_3$

$C_9H_{16}O_2 = 156.22$

Colorless liquid. B.P. 185° C. Sp.Gr. 0.887.

Almost insoluble in water, miscible with alcohol, essential oils and perfume and flavor chemicals.

Slightly pungent, fatty-fruity odor reminiscent of Pineapple, Rum, Arak, remotely of Peach. Less ethereal, but more natural Pineapple-like than Methyl caproate.

Fruity-fatty and vinous-sweet, Pineapple-like taste. Aqueous solutions of about 20 to 50 ppm should not show a pungent taste.

The ester finds some use in perfumery as part of a fruity topnote complex in fragrance types such as Miss Dior, Intimate, Cabochard, Ma Griffe, etc. In combination with green and mossy notes, it may form a characteristic part of such fragrance types. It also tends to round off the predominant Aldehyde-notes in combination with Styrallyl esters.

Originally a flavor material, it has found extensive use in Apple, Apricot, Arak, Orange, Peach, Pineapple, Rum, Strawberry, "Tutti-frutti", etc. It formed the major part of a "specialty" marketed under the name "Aldehyde C.20 – Pineapple".

Generally used as a modifier in fruit flavors (imitation).

Concentration: up to 30 ppm. in candy, and up to 200 ppm in chewing gum.

This chemical breaks down under alkaline conditions (soap) and may also be hydrolyzed in aqueous acid media (fruit flavors with acid), e. g. $p_H < 4$. This is one of its major drawbacks.

Produced by direct esterification of Allyl alcohol with Caproic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2032.

4-6; 23-Aug. 1949; 5-239; 26-394; 27-42; 34-1230; 77-186; 106-45; 140-141;

## 71: ALLYL CAPRYLATE

Allyl octylate.
Allyl octanoate.
Allyl octoate.
"Aldehyde C.19".
*2*-Propenyl octanoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_6{-}CH_3$

$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid. B.P. 222° C.
Sp.Gr. 1.005.

Insoluble in water, soluble in alcohol and oils.

Powerful fruity, slightly fatty Banana-Pineapple like odor with a somewhat oily-winey undertone.

Medium-sweet, fatty-fruity but not particularly pleasant flavor, unless tasted at the proper concentration (narrow limits of concentration). Quite natural Banana-Pineapple like in its overall character.

Rarely, if ever, used in perfumery.

Finds use in flavors as a modifier in imitation Pineapple, used in traces along with the Caproate and/or Caprinate, Amyl caprylate, Butyl caproate, etc.

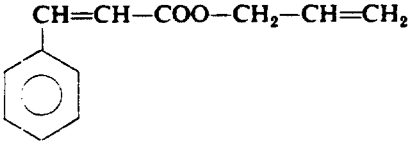
G.R.A.S. F.E.M.A. No.2037.

Produced by direct esterification of Allyl alcohol with Octanoic acid under azeotropic conditions.

B-I-734; B-II-384; 35-404; 4-6;

## 72: ALLYL CINNAMATE

Allyl-*beta*-phenylacrylate.
Propenyl cinnamate.
Vinyl carbinyl cinnamate.



$C_{12}H_{12}O_2 = 188.23$

Colorless or pale straw-colored, slightly viscous liquid. B.P. higher than 250° C.
Sp.Gr. higher than 1.00.

Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Weak, but tenacious Peach-Apricot type odor, winey, balsamic and somewhat Styrax-like.

NOTE: The product made by cross-esterification has an entirely different odor (usually carries considerable amounts of Methyl cinnamate).

Fruity-sweet, heavy Peach-Apricot type flavor.

Could find use in perfume types such as "Peachblossom" or Magnolia, etc.

Finds a little use in flavors, usually mere traces in fruit flavors.

Produced by direct esterification of Allyl alcohol with Cinnamic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2022.

B-IX(I)-230; 4-6; 47-296; 86-5;

## 73: ALLYL CYANIDE

*3*-Butene nitrile.
*beta*-Butenonitrile.
Vinyl acetonitrile.
Crotonic acid, nitrile.

$CH_2{=}CH{-}CH_2{-}CN$

$C_4H_5N = 67.09$

Colorless liquid. B.P. 119° C. Sp.Gr. 0.834.

Almost insoluble in water (the nitrile may hydrolyze), soluble in alcohol, miscible with essential oils and perfume chemicals.

Onionlike, but pleasant and rather sweet, not pungent.

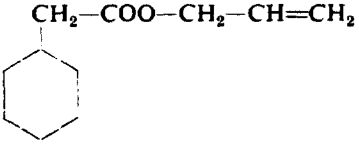
Could find use in imitation Onion flavors, Mustard compositions, etc. but it is not conceivable that this chemical would find much use in perfumery.

Produced from Allyl bromide plus Cuprous cyanide.

B-II-408; 100-36; 65-723; 66-635; 219-46; 160-794;

## 74: ALLYL CYCLOHEXANE ACETATE

Allyl cyclohexyl acetate.
Allyl hexahydro phenylacetate.



$C_{11}H_{18}O_2 = 182.27$

Colorless liquid, almost insoluble in water, miscible with alcohol, essential oils and flavor chemicals, perfume materials, etc.

Pronounced "mixed-fruity" odor, sweet, lasting and less ethereal than the lower aliphatic acetates.

The flavor is overall fruity ("tutti-frutti") with some resemblance to Pineapple, Peach and Apricot.

Could find use in perfumery as a softer fruity topnote – softer than Allyl caproate or Methyl phenyl carbinyl acetate, or as a modifier where other fruity materials are in use. Concentration would be about 0.5% to 2% in the perfume.

For imitation Pineapple flavors, this chemical could be used as a modifier with other "Pineapple" chemicals. Concentration in the finished (consumer) product would be about 10 ppm or less.

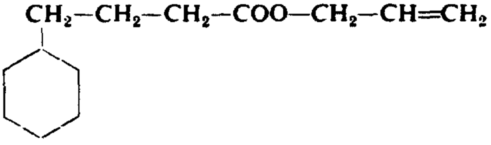
Produced by direct esterification of Allyl alcohol with Cyclohexaneacetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2023.

47-296; 140-144;

## 75: ALLYL CYCLOHEXANE BUTYRATE

Allyl cyclohexyl-*n*-butyrate.
Allyl hexahydrophenyl butyrate.



$C_{13}H_{22}O_2 = 210.32$

Colorless liquid. Insoluble in water, miscible with alcohol, essential oils, perfume and flavor chemicals.

"Mixed-fruity" odor of somewhat fatty character, quite tenacious.

Fatty Pineapple-like taste in acidified aqueous media.

Rarely, if ever, used in perfumes.

Traces are occasionally used in Pineapple as a modifier for Allyl cyclohexane propionate (imitation flavors).

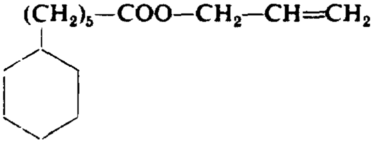
Produced by direct esterification of Allyl alcohol with Cyclohexane butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No. 2024.

47-296;

## 76: ALLYL CYCLOHEXANE CAPROATE

Allyl cyclohexyl hexoate.
Allyl hexahydro phenylcaproate.



$C_{15}H_{26}O_2 = 238.37$

Colorless liquid, insoluble in water, miscible with alcohol, essential oils and flavor chemicals.

Rather weak, fatty-fruity odor of considerable tenacity.

Weak, Peach-Apricot type flavor in aqueous media. Its effect is more perceptible when this chemical is used as a trace modifier with more volatile flavor chemicals.

Probably not used in perfumery.

Used in flavor compositions, but rarely. Mostly as a modifier for Allyl cyclohexane propionate. Traces of the caproate tends to mellow and round-off the sharper taste of the propionate.

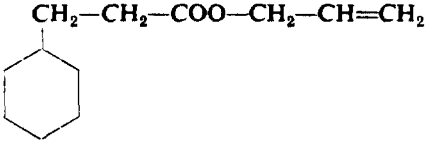
Produced by direct esterification of Allyl alcohol with Cyclohexane caproic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2025.

47-296;

## 77: ALLYL CYCLOHEXANE PROPIONATE

Allyl cyclohexyl propionate.
Allyl hexahydro phenylpropionate.
"Fruit ketone".
Allyl-*beta*-cyclohexyl propionate.
Allyl-*3*-cyclohexyl propionate.



$C_{12}H_{20}O_2 = 196.28$

Colorless, slightly oily liquid. Almost insoluble in water, miscible with alcohol, essential oils, perfume and flavor chemicals.
Sp.Gr. 0.95-0.97.

Powerful and sweet-fruity odor resembling Pineapple. Smoother and sweeter than Allyl caproate. Fruitiness similar to that of Linalyl-acetate.

Fresh-fruity sweet Pineapple-like taste.

Useful as a topnote ingredient in certain perfume types, also as a modifier for already existing materials: Allyl caproate, Linalyl-acetate, Methyl phenyl carbinyl propionate, Sweet Orange oil, etc.

More important in flavors: this chemical is often the chief carrier of the fruity note in imitation Pineapple, and an interesting modifier in imitation Strawberry, Raspberry, etc. A powerful fortifier in the popular "tutti-frutti" flavor types.

Concentration in perfumes: usually less than 1% of the composition. Concentration in flavors: 10 to 40 ppm in finished food products, somewhat higher in chewing gum and certain candies.

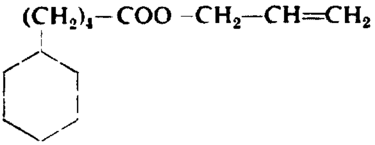
Produced by direct esterification of Allyl alcohol with Cyclohexanepropionic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2026.
E.O.A. No.254.

12-178; 47-296; 48-45 (erron. info.); 77-194; 86-5; DOW Chem. Co. orig. data sheet 1952; 140-144;

## 78: ALLYL CYCLOHEXANE VALERATE

Allyl cyclohexane pentanoate.
Allyl-*beta*-cyclohexyl valerianate.
Allyl hexahydrophenyl valerianate.



$C_{14}H_{24}O_2 = 224.35$

Colorless liquid. Insoluble in water, soluble in alcohol, essential oils, flavor materials, poorly soluble in Propylene glycol.

Heavy,sweet, mixed-fruity odor of great tenacity.

Peach-Apricot-Apple type flavor. In high dilution closer to Apple.

To the author's knowledge, not used in perfumery.

Occasionally used as a modifier for the propionate in imitation Pineapple (traces of the valerate), or in traces in Apple, Peach, Apricot, Mango and other imitation fruit flavors.

Concentration will usually be less than 5 ppm in the finished consumer product.

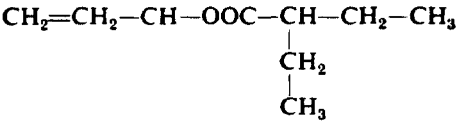
Produced by direct esterification of Allyl alcohol with Cyclohexanevaleric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2027.

47-296;

## 79: ALLYL-2-ETHYLBUTYRATE

*2*-Ethylbutyric acid, allyl ester.
*2*-Propenyl-*2*-ethylbutyrate.



$$CH_2{=}CH_2{-}CH{-}OOC{-}\underset{\substack{|\\ CH_2\\ |\\ CH_3}}{CH}{-}CH_2{-}CH_3$$

$C_9H_{16}O_2 = 156.23$

Colorless liquid. B.P. approx. 186° C.

Insoluble in water, miscible with alcohol, essential oils, flavor materials.

Peculiar oily-fruity odor, nondescript fruit type.

Fruity, oily-nutlike taste, faintly resembling the pit of cherry, peach or plum, but not exactly almondy. The oily-nut-like notes are characteristic of many aliphatic C-9 materials.

This material could find use in flavors for imitation Apricot, Peach, Pineapple, Cherry and many other fruit flavors. Its peculiar aroma limits its use concentration to mere traces in the composition.

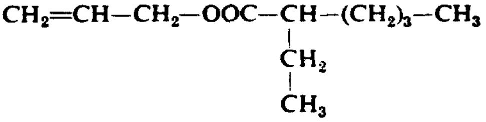
Produced by direct esterification of Allyl alcohol with 2-Ethylbutyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2029.

47-296;

## 80: ALLYL-2-ETHYLHEXOATE

Allyl ethylcaproate.
*2*-Ethylcaproic acid, allyl ester.
*2*-Propenyl ethylcaproate.
Allyl-*iso*-caprylate.
Allyl ethylbutylacetate.
Allyl-*alpha*-ethyl-*n*-caproate.
Allylheptane-*gamma*-carboxylate.



$$CH_2{=}CH{-}CH_2{-}OOC{-}\underset{\substack{|\\ CH_2\\ |\\ CH_3}}{CH}{-}(CH_2)_3{-}CH_3$$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. B.P. approx. 190° C.
Sp.Gr. 0.863.

Almost insoluble in water, miscible with alcohol and essential oils, perfume and flavor chemicals.

Sweet and fruity odor without having characteristics of any specific type of fruit.

Somewhat woody-fruity, slightly nut-like, peach-kernel like flavor.

Probably not used in perfumery.

Used in traces in imitation Pineapple, Peach. Apricot and other fruit flavors, often as a modifier for Nonalactone-Undecalactone or other materials used to introduce fatty-pit-like notes.

Produced by direct esterification of Allyl alcohol with 2-Ethylcaproic acid under azeotropic conditions.

NOTE: the isomer, Allyl caprylate, is G.R.A.S. (specified). This particular chemical is not listed as G.R.A.S.

47-296;

## 81: ALLYL FORMATE

Propenyl formate.
Vinyl carbinyl formate.
2-Propenyl methanoate.

$CH_2{=}CH{-}CH_2{-}OOCH$

$C_4H_6O_2 = 86.09$

Colorless mobile liquid. B.P. 83° C.
Sp.Gr. 0.948.

Slightly soluble in water, soluble in alcohol and oils.

Ethereal-fruity odor, slightly pungent and, in moist atmosphere, reminiscent of Mustard. However, this phenomenon may well be a result of instant hydrolysis of this fragile ester.

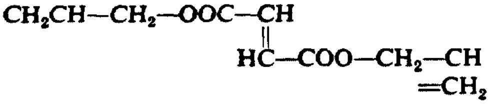
For the above reason, it is not likely that this chemical will find much use in flavors.

Produced by direct esterification of Allyl alcohol with Formic acid under azeotropic conditions (water-carrier must be very low-boiling).

26-394; 66-544; 86-5; B-II-23; 160-1000;

## 82: ALLYL FUMARATE

Diallyl fumarate.
Diallyl-*trans*-butene dioate.



$$\begin{array}{l} CH_2CH{-}CH_2{-}OOC{-}CH \\ \qquad\qquad\qquad\qquad\quad \| \\ \qquad\qquad\qquad\qquad HC{-}COO{-}CH_2{-}CH \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad {=}CH_2 \end{array}$$

$C_{10}H_{12}O_4 = 196.21$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Peculiar sweet-musty, fungal, Champignon-like odor.

Sweet mushroom-like, musty, "overfermented" taste.

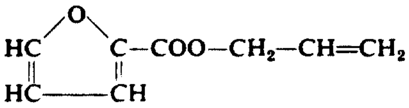
This ester has been suggested for use in flavor compositions for imitation Champignon (mushroom) and other fungoid flavors.

Prod.: from Fumaric acid and Allyl alcohol.

77-189;

## 83: ALLYL-2-FUROATE

Pyromucic acid, allyl ester.
Allyl furan-*2*-carboxylate.



$C_8H_8O_3 = 152.15$

Colorless or pale straw-colored liquid. Darkens when exposed to daylight or air.

Very slightly soluble in water, miscible with alcohol, essential oils, flavor chemicals, and soluble in Propylene glycol.

Caramellic-fruity odor, often classified as "jam-like" or "cooked-preserve-like", reminiscent of canned, syrypy fruit.

Fruity-pineapple-strawberry-like flavor with a distinct note toward the caramellic (according to purity of the chemical).

Useful in flavors for imitation Pineapple, Strawberry, Mango, etc. in traces (mostly less than 1 ppm in the finished food). Interesting in imitation – or "reconditioned" Coffee flavor.

G.R.A.S. F.E.M.A. No.2030.

86-5; 140-174;

## 84: ALLYL HEPTIN CARBONATE

Allyl heptin carboxylate.
Allyl-*2*-octynoate.
Allyl amylacetylene carboxylate.
*2*-Propenyl amylacetylene carboxylate.

$CH_2{=}CH{-}CH_2{-}OOC{-}C{\equiv}C{-}(CH_2)_4{-}CH_3$

$C_{11}H_{16}O_2 = 180.25$

Colorless oily liquid. Insoluble in water, soluble in alcohol and perfume materials, poorly soluble in Propylene glycol.

Very powerful, but quite natural and not very pungent green-leafy, violet-leafy odor, typical "foliage" odor, less gassy than the Methyl ester.

Could be used in perfumery as a variant for green-leafy topnotes, but its character is primarily that of Violet-leaf. It almost demands to be accompanied by Ionones.

In mere traces, about 0.1%, it may introduce quite pleasant and unusual lift to single florals. In non-floral compositions, it blends well with sweet-fruity notes. Ylang-Ylang extra is, therefore, an ideal companion to this chemical. Oakmoss, on the other hand, can make good use of traces of Allyl h-c.

Produced from Castor oil via Heptaldehyde – Heptyne – which is treated with Allyl-chlorcarbonate and Sodium to yield Allyl-h-c.

## 85: ALLYL HEPTOATE

Allyl heptanoate.
Allyl heptylate.
Allyl oenanthate.
Propenyl heptoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_5{-}CH_3$

$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. Insoluble in water, miscible with essential oils and perfume materials, poorly soluble in Propylene glycol.

B.P. 210° C. Sp.Gr. 0.890.

Sweet-fruity, somewhat pungent, vinous Banana-like odor.

Heavy-vinous, Apricot-Brandy-Peach-Pineapple-like flavor.

Occasionally used in floral fragrance compositions: Appleblossom, Peachblossom, Magnolia, Sweet Pea, etc.

More frequently used in flavors for imitation Apricot, Berry, Brandy, Peach, Pineapple etc. In Europe occasionally for Gooseberry.

Concentration usually about 2-7 ppm. in finished consumer product, except in chewing gum – up to 800 ppm.

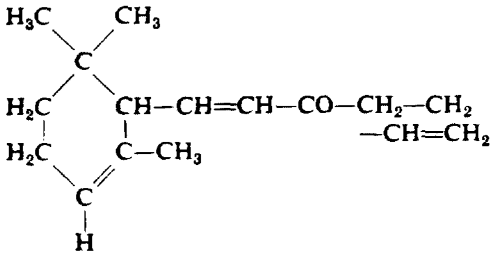
Produced by direct esterification of Allyl alcohol with Heptanoic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2031.

35-61; 86-5; 77-187; 140-142;

## 86: ALLYL IONONE

*alpha*-Allyl ionone (Allyl-*alpha*-ionone).
"Hexalon" (I.F. & F. Inc.).
"Cetone V." (Givaudan).
"Polyone" (Firmenich).
Allyl cyclocitrylidene acetone.
*1*-(*2*,*6*,*6*-Trimethyl-*2*-cyclohexene-*1*-yl)-*1*,*6*-heptadien-*3*-one.



$C_{16}H_{24}O = 232.35$

Colorless or very pale yellowish oily liquid. B.P. about 265° C. Sp.Gr. 0.930.

Oily-sweet, slightly flowery, but also fruity, woody and bark-like green odor of considerable tenacity. According to the identity of the manufacturer, the odor characteristics of this chemical may vary from mild-oily fruity-woody to peculiar fishy (amine-like), woody, cod-liver oil-like, etc. The odor changes also with age, particularly under poor storage conditions. This is one of the main drawbacks of the title chemical.

Ketone content of commercial grades: 88 to 93%.

Insoluble in water, soluble in alcohol and perfume and flavor materials, poorly soluble in Propylene glycol.

Useful in perfume compositions as a modifier for Ionones and Methylionones, in modern-aldehydic creations, in perfumes with fruity-aldehydic topnotes, in combinations with Vetiver or woody-floral perfume materials, etc. "Cetone V." is probably the most fruity of all commercial Allyl ionones.

Used in flavors – in traces – for imitation Raspberry and Pineapple.

Produced from Citral by condensation with Allyl acetone, followed by cyclization.

G.R.A.S. F.E.M.A. No.2033.

3-171; 31-96; 86-5; 106-94; 155-92; 89-389; 156-203;

## 87: ALLYL MERCAPTAN

Allyl thiol.
Allyl sulfhydrate.
*2*-Propene-*1*-thiol.

$CH_2{=}CH{-}CH_2{-}SH$

$C_3H_6S = 74.14$

Colorless mobile liquid. B.P. 90° C. Sp.Gr. 0.925.

Almost insoluble in water, miscible with alcohol and oils.

Penetrating and extremely diffusive onion-like, but sweet and not really pungent odor. Not a lachrymator. Odor also resembles that of leek.

This chemical finds some use in combination spice flavors, particularly for soups and meat. It is used in mere traces in such flavor compositions.

Produced from Allyl bromide and Potassium hydrosulfide.

G.R.A.S. F.E.M.A. No.2035.

B-I-440; 26-394; 66-347;

## 88: ALLYL NONANOATE

Allyl pelargonate.
Allyl nonylate.
*2*-Propenyl nonanoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_7{-}CH_3$

$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid. B.P. approx. 230° C.

Insoluble in water, soluble in alcohol, miscible with essential oils, perfume and flavor chemicals.

Fruity-winey, somewhat fatty-oily odor, resembling that of wine residue, cognac residue or the like. A trace of sharpness in the fruity notes resembles Pineapple.

In slightly acidified sugar solution, the taste is at the same time brandylike, Cognac, and Pineapple-fruity.

Apparently, this ester finds very little use in perfumery, although it could be applied with advantage as a topnote ingredient to round off aldehydic or overly green notes in modern fragrance types.

This chemical finds some use in flavor compositions, in imitation fruit flavors, artificial Cognac, Rum, Wine, and in artificial "Cognac oil". It is applied in mere traces.

Prod. by direct esterification, from Allyl alcohol and Nonanoic acid, using azeotropic distillation to remove water.

G.R.A.S. F.E.M.A. No.2036.

47-296; 140-143;

## 89: ALLYL-2-NONYLENATE

*2*-Propenyl-*2*-nonylenate.
Allyl nonenoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}CH{=}CH{-}(CH_2)_5{-}CH_3$

$C_{12}H_{20}O_2 = 196.29$

Colorless oily liquid. Insoluble in water, soluble in alcohol, miscible with ess. oils and flavor chemicals.

B.P. approx. 262° C.

Fatty and slightly nutty, green-fruity, somewhat Pineapple-like odor.

Fatty-oily, Pineapple-fruity taste. Quite powerful.

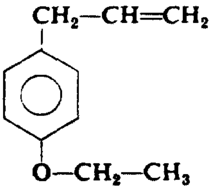
This ester could find use in flavor compositions, although it is less versatile than the saturated ester (Allyl nonanoate). In traces in Pineapple imitation as a modifier, and to introduce fruity-oily notes in Rum and Arak imitation flavors.

Prod. by direct esterification of Allyl alcohol with Nonenoic acid, under azeotropic conditions.

47-296;

## 90: para-ALLYL PHENETHOLE

Ethyl chavicol.
Chavicol ethylether.
*para*-Ethoxy propenyl benzene.
*4*-Ethoxy-*1*-allyl benzene.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid. B.P. 232° C.
Sp.Gr. 0.955.

Weak, anisic, sweet odor, more pungent than Anethole, less sweet or mild.

Somewhat medicinal-sweet or spicy taste.

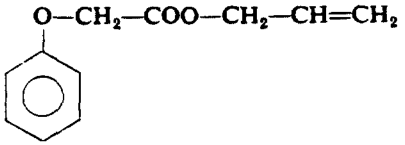
This ether could find use in perfumes as a sweetening fixative or as a modifier for Estragole (Methyl chavicol).

Prod. by ethylation of Chavicol with Diethyl sulfate.

31-150; 72-38; 90-392 (Methyl ether); 90-426 (Methyl ether).

## 91: ALLYL PHENOXYACETATE

"Acetate P.A.".



$C_8H_8O_3 = 152.15$

Colorless liquid. B.P. approx. 265° C.

Somewhat sharp, mixed-fruity, mainly Pineapple-like and honey-sweet odor of great tenacity.

Heavy-sweet fruity-honey-like taste, somewhat reminiscent of "cooked" fruit.

Rarely, if ever, used in perfumery, except for "honey"bases, etc.

Used in flavor compositions, as a modifier in imitation Strawberry, Pineapple, etc. in mere traces.

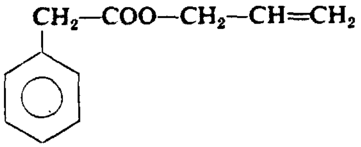
Prod. by direct esterification of Allyl alcohol with Phenoxy acetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2038.

12-178; 47-296; 50-359;

## 92: ALLYL PHENYLACETATE

*2*-Propenyl phenylacetate.



$C_{11}H_{12}O_2 = 176.22$

Colorless slightly viscous liquid.
B.P. approx. 230° C.

Insoluble in water, miscible with alcohol and oils.

Sweet honeylike, but faint odor with sweet-fruity undertones and good tenacity. Less floral than the Phenoxy-ester.

Honey-like taste.

Finds limited use in perfumery as a component of "honey" bases ("miel", etc.) along with other esters of Phenylacetic acid and Phenoxy acetic acid.

Used in flavor compositions as a modifier with other Phenylacetates in imitation Pineapple, Honey and various fruit or Rum flavors. Concentration up to 40 ppm in baked goods (finished prod.). Its honey-like aroma is also utilized in tobacco flavoring.

Produced by direct esterification of Allyl alcohol with Phenylacetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2039.

47-296; 77-194; 86-5; 4-6;

## 93: ALLYL PROPIONATE

*2*-Propenyl propionate.

$CH_2{=}CH{-}CH_2{-}OOC{-}CH_2{-}CH_3$

$C_6H_{10}O_2 = 114.14$

Colorless liquid. B.P. 124° C.

Somewhat sharp, sour-fruity odor, suggestive of Apple and Apricot.

Fresh and light, ethereal-fruity taste of somewhat sour type, reminiscent of Apple, Apricot and Pear.

Useful in imitation fruit flavors of the "sour" type, such as: Apple, Apricot, Gooseberry, Peach, Pear, Pineapple, Plum, etc.

Concentrations up to 15 ppm in Ice Creams (finished product).

Prod. by direct esterification of Allyl alcohol with Propionic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2040.

26-396; 47-296; 86-5; B-II-141;

## 94: ALLYL PROPYL DISULFIDE

$CH_2{=}CH{-}CH_2{-}S{-}S{-}CH_2{-}CH_2{-}CH_3$

$C_6H_{12}S_2 = 148.28$

Almost colorless or pale yellowish liquid. B.P. approx. 170° C.

Powerful onionlike-garlic-like odor. Not pungent, more garlic-like than onionlike (NOT a lachrymator).

This chemical, which occurs in natural food products, could find use in flavor reconstitution of soups, meat preserves, etc. in spice blends, sausages, etc.

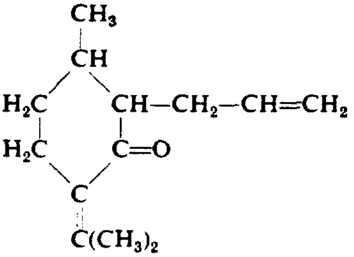
To the author's knowledge, this chemical is not offered commercially at the present time (1968).

It is conceivable that it would be permissible in flavor compositions for food products, since it occurs in Garlic, Onion and Asafoetida oils.

65-731; 90-827; 61-Nov.-53; 158-136;

## 95: ALLYL PULEGONE

*2*-Allyl-*para*-menthene-(*4*(*8*))-one-*3*.
*1*-Methyl-*2*-allyl-*4*-*iso*-propylidene cyclohexanone-*3*.
(exists in *laevo*- and *dextro*-form, the *laevo*- being described below).



$C_{13}H_{20}O = 192.30$

Colorless or pale yellowish oily liquid.
B.P. approx. 230° C. Sp.Gr. 0.94.

Sweet-woody odor reminiscent of Ionones, Cedarwood and Vetiver, quite pleasant and fairly tenacious.

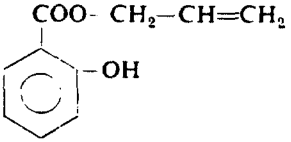
Although not widely known and appreciated this material could find use as a modifier and fixative-blender in Oriental type fragrances, Rose, Violet and Wood compositions.

Prod. from Pulegone, isolated from Pennyroyal oil.

7-21; 31-89; B-II, Erganz. bd. 7-139;
see also: *1*-Methyl-*2*-propenyl-*4*-*iso*-propylbenzene.

## 96: ALLYL SALICYLATE

*2*-Propenyl salicylate.
*2*-Propenyl-*ortho*-hydroxybenzoate.



$C_{10}H_{10}O_3 = 178.19$

Colorless liquid. B.P. 248-250° C.
Sp.Gr. 1.10.

Peculiar herbaceous-fruity odor, softer than Amylsalicylate, slightly more fruity, not as harsh. A faint undertone of "Wintergreen" character.

Fruity-herbaceous taste, reminiscent of Grape, Wintergreen, Banana and Pineapple.

This ester could find some use in perfumery, but it does add a certain amount of hazard in that both components (acid and alcohol) are harmful to the human skin.

The material is NOT listed in the American G.R.A.S. list for food chemicals, materials and additives, and it is doubtful whether this chemical will find use as a food flavor.

Prod. by direct esterification of Allyl alcohol with Salicylic acid under azeotropic conditions.

This chemical appears quite frequently in the perfume chemistry literature, but the author does not find this abunhance of mention synonymous with popularity as a perfume or flavor chemical.

7-21; 31-134; 34-788; 47-296; 86-5; 95-188;

## 97: ALLYL SORBATE

Allyl-*2,4*-hexadienoate.
*2*-Propenyl sorbate.

$$CH_2{=}CH{-}CH_2{-}OOC{-}CH{=}CH{-}CH{=}CH{-}CH_3$$

$$C_9H_{12}O_2 = 152.20$$

Colorless liquid. Tends to polymerize, becomes viscous and finally solid, odorless, unless properly stabilized with inhibitor.

Pungent-fruity, diffusive, Pineapple-like, sweet odor.

Sweet, Melon-like, Pineapple-like, almost anisic-fruity taste.

This material is, to the author's knowledge, not used in perfumery.

It finds some use in flavor compositions for imitation fruit flavors, in which it is applied in mere traces.

Prod. by direct esterification of Allyl alcohol with Sorbic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2041.

12-178; 47-296; 50-359;

## 98: ALLYL-iso-THIOCYANATE

Allyl-*iso*-rhodanide.
Allyl Mustard oil.
Mustard oil, artificial.
Allyl-*iso*-sulfocyanate.
Allyl senevol.
Allyl thiocarbonimide.

$$CH_2{=}CH{-}CH_2{-}N{=}C{=}S$$

$$C_4H_5NS = 99.15$$

Colorless mobile liquid. B.P. 151-153° C. Sp.Gr. 1.025.

Slightly soluble in water, miscible with alcohol and flavor materials. The oil turns darker yellow upon exposure to air and daylight.

Extremely penetrating, pungent and stinging odor. This chemical is a powerful lachrymator, and inhalation of its vapors may cause serious damage to human lungs. The liquid and its vapors produce blisters on the human skin. A few grams may kill a man, if the oil is taken internally.

In spite of its apparent power and pungency, this chemical can be tolerated in surprisingly high concentration as a flavor chemical. However, the pungency is perceptible down to a level of 1-3 ppm in aqueous solution.

Used quite extensively in flavor compositions, particularly along with vinegar (pickled products). Also in meat and spice flavors. Concentration in pickled products may be as high as 80 ppm.

This chemical is very unstable. It is decomposed under influence of air, light, water, metals, etc. and even alcoholic solutions are unstable.

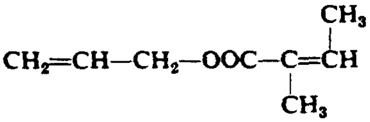
Prod. from Allyl iodide and Potassium sulfocyanide. This chemical is the chief component of the volatile oil of black Mustard seed, and can be isolated by enzymatic breakdown of the glycoside in the seed.

G.R.A.S. F.E.M.A. No.2034.

3-115; 7-21; 65-734; 66-946; 72-27; 77-213; 85-106; 86-123; 90-841; 100-37; 140-177; 160-1066;

## 99: ALLYL TIGLATE

Allyl-*trans*-*2*-methyl-*2*-butenoate.
Allyl tiglinate.
*see NOTE.



$$CH_2{=}CH{-}CH_2{-}OOC{-}\underset{CH_3}{C}{=}\overset{CH_3}{C}H$$

$C_8H_{12}O_2 = 140.18$

Colorless liquid. Very slightly soluble in water, miscible with alcohol and oils.

Mild, herbaceous-fruity odor with a faint green note.

Sweet-fruity, rather mild and non-descript flavor.

This chemical finds some use in flavor compositions, mainly in imitation fruit flavors. It is used in mere traces.

Prod. by direct esterification of Allyl alcohol with Tiglic acid under azeotropic conditions.
*NOTE: Commercial Tiglic acid has for some time been marketed as a mixture of Tiglic and Angelic acids. It is most conceivable that many esters named – tiglate are actually mixtures of -tiglate and -angelate.

G.R.A.S. F.E.M.A. No.2043.

4-6;

## 100: ALLYL UNDECYLATE

*2*-Propenyl hendecanoate.
NOTE: The most common commercial product is the ester of the unsaturated acid: Allyl undecylenate, and the name Allyl undecylate is frequently applied in error to that chemical.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_9{-}CH_3$

$C_{14}H_{26}O_2 = 226{,}36$

Colorless oily liquid. BP. 260° C.
Sp.Gr. 0.895.

Vinous-fruity, fatty and powerful Banana-Pineapple type odor with Coconut-like background. Also reminiscent of Peach and Mango.

Powerful fruity and oily-sweet Peach-Pineapple type flavor.

Finds a little use in perfumery as a fruity fixative or as a fruity note in the fixative portion of perfume creations.

Used in flavors for imitation Rum and Fruit-Rum combination flavors.

Prod. by direct esterification of Allyl alcohol with Undecylic acid under azeotropic conditions.

35-854; 47-296;

## 101: ALLYL UNDECYLENATE

*2*-Propenyl undecenoate.
Allyl-*10*-undecenoate.

$CH_2{=}CH{-}CH_2{-}OOC{-}(CH_2)_8{-}CH{=}CH_2$

$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. B.P. 230° C.
Sp.Gr. 0.935.

Insoluble in water, soluble in alcohol, miscible with essential oils, perfume and flavor materials.

Fatty, Coconut-Pineapple type odor, powerful Rum-like background, reminiscent of Rum-residue, heavy, oily-sweet.

Fatty Pineapple-like, sweet (in extreme dilution), nutlike taste, reminiscent of Cocoabean and Coconut.

Rarely, if ever, used in perfumes.

Useful in flavor compositions of fruity Rum type, nutty-coconutty imitation flavors, etc. Concentration will usually be a few ppm or less in the finished consumer product.

Prod. by direct esterification of Allyl alcohol with Undecylenic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2044.

35-854; 47-296; 86-5; 101-4 (Th.St.Just, Manchester, info.sheet).

## 102: ALLYL-iso-VALERATE

*2*-Propenyl-*iso*-valerate.
Allyl-*iso*-valerianate.

NOTE: This material is occasionally offered commercially under the name Allyl valerate. To the author's knowledge, the *normal*-Valerate is NOT used in perfumes or flavors.

$CH_2{=}CH{-}CH_2{-}OOC{-}CH_2{-}CH(CH_3)_2$

$C_8H_{14}O_2 = 142.19$

Colorless liquid. B.P. 155° C.
Sp.Gr. slightly above 1.00.

Insoluble in water, soluble in alcohol, miscible with perfume and flavor materials. Poorly soluble in Propylene glycol.

Powerful winey-fruity, "fermented", Apple-like odor.

Fruity Apple-like taste, somewhat sharp, berry-like.

Rarely, perhaps never, used in perfumes.

Useful in flavor compositions for imitation Apple, Cherry, Pear, Pineapple, etc.

Concentration up to 50 ppm in baked goods (consumer product). Much lower in liquid products.

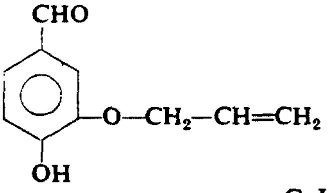
Prod. by direct esterification of Allyl alcohol with *iso*-Valeric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No. 2045.

86-5; 26-396; 49-136; B-II-313; 160-1068;

## 103: ALLYL VANILLIN

*3*-Allyloxy-*4*-hydroxybenzaldehyde.
Protocatechualdehyde-*3*-allylether.



$C_{10}H_{10}O_3 = 178.19$

White crystals of Vanillin-like odor, somewhat weaker than Vanillin, but also more natural Vanilla-like.

Pleasant Vanilla-type taste, softer than that of Vanillin, and not quite as powerful.

This chemical could find use as a modifier to accompany Vanillin and/or Ethylvanillin (so-called) in all flavor types where Vanillin-type flavor is called for.

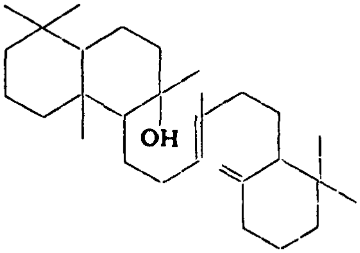
However, since Allyl vanillin is not readily available, there is little chance of its becoming a popular flavor chemical.

Prod.: among several methods, the preparation of Protocatechualdehyde from Safrole, followed by Alkylation with Allyl bromide will yield Allyl vanillin.

12-119; 86-133; 140-279;

## 104: AMBREIN

A triterpenoid *tertiary*-alcohol.
Do not confuse with the "Ambrain" derived from Labdanum gum.



$C_{30}H_{52}O = 428.75$

The title material is briefly mentioned in this work, because it represents a milestone in the perfume chemistry research (connected with Vitamin- and Hormone-research). It may also serve to further elucidate monographs and materials as mentioned under the title: Sclareol or under the monograph: Abietic acid.

Ambrein is an odorless solid material, but it is a parent of numerous very important Ambregris perfume materials, including those produced in Nature.

Oxidation products of Ambrein have been manufactured, and thus opened the door to partial synthesis of the Ambregris odor. One commercial product (Ambrone T or Ambrone clair, Takasago Perfumery Co. Ltd., Japan) is manufactured by way of ozonolysis of odorless Ambrein and concentration of the odorous, volatile oxidation products.

Since natural Ambregris contains substantial amounts of odorless Ambrein, the ozonolysis method leads to an increased "yield" of perfumery grade odorous Ambregris material. Mother Nature's incomplete synthesis has been helped to completion by man.

Among the odorous derivatives from Ambrein are:

Ambrenolide (Lactones $C_{16}H_{26}O_2$), Decalin-derivatives.

Ambrinols – liquid or solid, *tertiary*-alcohols (Octalin-derivatives).

Cyclo homogeraniol and related materials.

Dihydro-*gamma*-ionone.

Cyclopropan derivatives.

Various epoxides and aldehydes.

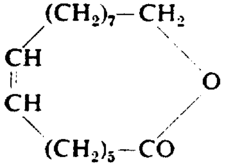
The literature on the subject of Ambrein is less than 30 years old, and yet very abundant. Interested readers will find ample information in specialized works on the subject.

67-744; 87-400; 88-367; 163-171; 163-322; "The Givaudanian", May 1959, page 4.

See monograph: Sclareol.

## 105: AMBRETTOLIDE

Cyclohexadecen-*7*-olide.
*16*-Hydroxy-*Δ7*-hexadecenoic acid, lactone.
"Moskus Lakton".
*16*-Hydroxy-*1*-hexadecenoic acid, lactone.



$C_{16}H_{28}O_2 = 252.38$

Colorless, somewhat viscous oil with rich and extremely tenacious floral-musky, sweet odor. B.P. about 300° C. Sp.Gr. 0.958.

Soluble in alcohol and oils.

This chemical is one of the finest fixatives among the distinguished group of those showing a synergistic and amplifying effect upon perfumes and flavors. At the same time it increases the diffusiveness of fragrances in which it is incorporated. Its fixative effect is easily recognized by the fact that solutions of 0.01% Ambrettolide (or even less) in slightly diluted alcohol show practically no odor of alcohol, only a faint, floral-musky, sweet and pleasant odor of the lactone. A. is particularly useful in fragrance types of delicately floral, mildly animal or Ambre-like type.

A. finds extensive use – in extremely low concentration – as a modifier-blender ("ageing-mellowing" agent) in flavor compositions, particularly in alcoholic beverages. Its effect is easily perceptible at concentrations below 0.01 ppm. (less than one part in one hundred million parts of finished product). Concentrations up to 0.7 ppm are known in certain consumer products, fruit flavors, etc.

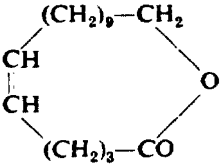
Prod.: Many patented methods are known, few are commercially feasible. From Bromo hexadecenoic acid, or from Dihydroxy palmitic acid, or from Aleuritic acid, or from Juniperic acid, etc.

G.R.A.S. F.E.M.A. No.2555.

5-203; 27-43; 30-271; 31-178; 86-10; 106-46; 90-670; 156-250; 37-716; 159-437; 159-632; GIVAUDAN data sheet 1962 (Dr. Ch. Collaud, Givaudan – Geneva).

## 106: $\Delta^5$-iso-AMBRETTOLIDE

Cyclohexadecen-*5*-olide.



$C_{16}H_{28}O_2 = 252.38$

Colorless oily liquid.

Faint, musky odor, weaker than Ambrettolide.

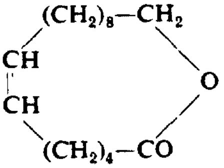
Beyond its limited academic interest in the study of macrocyclic lactones and Musk odor, this chemical has little, if any application in practical perfumery or flavor work.

Prod. from *16*-Hydroxy-$\Delta^5$-hexadecenoic acid by lactonization.

5-205;

## 107: $\Delta^6$-iso-AMBRETTOLIDE

Cyclohexadecen-*6*-olide.



$C_{16}H_{28}O_2 = 252.38$

Colorless oily liquid.

Faint, musky odor, weaker than Ambrettolide.

Little or no interest beyond the academic. Probably not used in perfumery and, or flavor work.

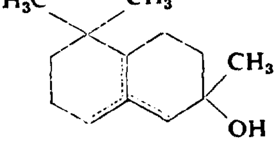
Prod. from *16*-Hydroxy-$\Delta^6$-hexadecenoic acid by lactonization.

5-205;

## 108: AMBRINOL

Ambrinol or Ambrinols are a group of isomer Octalin derivatives of the general formula and structure:

*2,5,5*-Trimethyl-*2*-hydroxy-octalin.



$C_{13}H_{22}O = 194.32$

Isomers with the unsaturation (double bond) in positions 8, 9 or 1,9 are the three materials of particular interest to perfumery.

Colorless liquids, or white solid materials of M.P. 60-70° C.

The title materials are briefly mentioned in this work because of their potential interest to the perfumer. They are natural components of Ambregris, and they are considered of major importance to the olfactory properties of natural Ambregris and Ambregris tincture.

Although the materials have been synthesized, and also obtained as isolates from natural Ambregris, they are not yet commercially available under the name Ambrinol. Closely related chemicals are made synthetically at lower cost, but not of the same attractive olfactory effect.

The eyecatching similarity in structure

between Ambrinols and Ambrein, Sclareol, Abietic acid and Dihydro-*gamma*-ionone, etc. has been the subject of much discussion in modern perfumery literature.

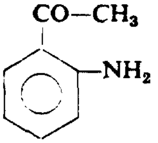
When the title materials become commercially available at an attractive price, they will undoubtedly find their way into perfumery as part of Ambre bases, new perfume types, specialties, etc. Certain specialties are already partly based upon the use of the title materials.

163-323;

See also monographs:
Abietic acid.
Ambrein.
*gamma*-Cyclohomogeraniol.
Dihydro-*gamma*-ionone.
Manool.
Sclareol.
Tetramethyl octalyl ethanal.
Tetramethyl octalyl ethanol.
Squalene,
etc. (see footnote under Sclareol).

## 109: ortho-**AMINOACETOPHENONE**

*1*-Acetyl-*2*-aminobenzene.



$C_8H_9NO = 135.16$

B.P. 250° C. (decompos.).

Colorless or pale yellowish liquid. Darkens when exposed to daylight or air.

Soluble in alcohol and perfume materials. Insoluble in water.

Heavy-sweet, somewhat animal-floral odor of considerable tenacity, faintly reminiscent of tobacco leaf odor.

This chemical has found some use as a modifier in Jasmin bases and Jasmin perfumes.

Prod.: (several methods) e. g. by controlled reduction of *ortho*-Nitroacetophenone. Also from *ortho*-Aminophenylpropiolic acid.

3-214; 4-241; 26-396; 68-1014; B-XIV-41;

## 110: alpha-**AMINOBUTYRIC ACID**

$CH_3—CH_2—CH(NH_2)—COOH$

$C_4H_9NO_2 = 103.12$

White crystalline powder.

Melting point for *dl*-form: 285° C. (decompos.).

Soluble 33% in cold water, poorly in alcohol, insoluble in oils. In the dry state, this chemical has only a very faint caramellic-sweet odor.

When applied in combination with Glucose, it produces a flavor reminiscent of Maple sugar.

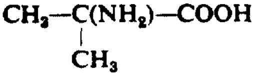
Finds considerable use in flavor work. It is a commercially available Maple flavor material.

Prod.: Can be isolated from natural proteins. It is present in the tendon of the sperm whale and along with many other animal proteins.

Synthetic: from Acetone (Blatt: Org. Synth. Coll. vol. II, page 29. New York 1943) or by the Bucherer method (Org. Synth. vol. XX 1940, page 42).

51-50; 66-829; 58-March-54; 60-May-59; 26-398; B-IV-408;

## 111: alpha-AMINO-iso-BUTYRIC ACID



$CH_3—C(NH_2)—COOH$ with $CH_3$ below

$C_4H_9NO_2 = 103.12$

White prismatic or leafy crystals.

Very easily soluble in water, poorly soluble in alcohol, insoluble in oils.

Melting point: 203° C. (under decomposition).

Practically odorless in the dry state.

When fused with Glucose, it produces an odor similar to that of Maple sugar.

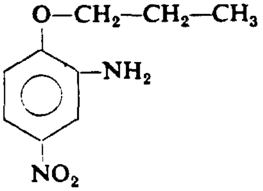
Finds use in flavor compositions for its Maple-like flavor when treated with Glucose under heating.

Prod. from Acetone (Blatt: Org. Synth. Coll. vol. II, page 29, 1943) or by the Bucherer method (Org. Synth. vol. XX, 1940, page 42).

26-398; 66-829; 58-March-54; 60-May-59; B-IV-414;

## 112: 2-AMINO-4-NITRO-1-n-PROPOXY BENZENE

*4*-Nitro-*2*-aminophenyl propylether.



$C_9H_{12}N_2O_3 = 196.21$

Orange-colored crystals. M.P. 48° C.

Very poorly soluble in water, slightly soluble in alcohol and some oils.

Virtually odorless when pure. Commercial products often have a slightly sweet-musty, bland odor.

The subject material is one of the sweetest substances known. Its sweeting power is estimated at 3,300 to 4,100 times that of cane sugar.

A saturated aqueous solution, containing 0.0136% of this material, equals a 50% cane sugar solution in sweetness.

Although this chemical is related to Dulcin, which has been removed from food additives many years ago (1950, see monograph: Dulcin), it has not yet been banned from use in food.

The very powerful sweeteners all suffer from the economic ailment, that the possible volume of total sales and use of such chemicals is far too small to tempt the chemical industry to make the material. It is therefore most conceivable that modern research aiming at artificial sweeteners will be concentrated upon the "medium-strong" sweeteners of a power equal to 30 to 60 times that of cane sugar. And it has become a popular practice to use a combination of a high-power plus a low-power sweetener in the best-selling consumer products.

It is surprising to notice that subject chemical – according to some observers – has anaesthetic effect. Although this is not uncommon among alkylated Aminophenols, it is hard to understand how the material at the same time can be the most powerful sweetener known.

Higher and lower homologues of subject chemical have all lower sweetening effect:

| | |
|---|---|
| Methyl ether: | 220 times cane sugar |
| Ethyl ether: | 950 times cane sugar |
| *iso*-Propylether: | 600 times cane sugar |
| *n*-Butyl ether: | 1000 times cane sugar |
| Allyl ether: | 2000 times cane sugar |

Prod.: by Alkylation of *ortho*-Amino-*para*-nitrophenol.

30-318; 30-320; 161-328;
see also: Chemical & Engineering News, vol. 44, Oct. 10, 1966, page 108/112.

## 113: AMMONIUM CARBONATE

Hartshorn. (folksname).
"Smelling salt".
Commercial product is a mixture of:
Ammonium bicarbonate: $NH_4HCO_3$ and
Ammonium carbamate: $NH_2$—$COONH_4$.
The mixture contains approximately 30 to 33% $NH_3$.

Colorless crystalline mass or white powder or translucent lumps. Soluble in water (about 20% in cold water), but decomposes in hot water.

Ammonium carbamate is soluble in alcohol, the bicarbonate is not. Strong odor of Ammonia, somewhat alkaline taste.

Used in baking powder, and has been used as a smelling salt, now practically abandoned.

Although Ammonia is considered somewhat toxic, this chemical is tolerated to a considerable degree by the human system. Quantities up to 2.0 grams in a 24-hour period have been given internally for medicinal purposes.

Prod. by subliming a mixture of Calcium carbonate and Ammonium sulfate.

100-64; (Food Chemicals Index);

## 114: AMMONIUM CHLORIDE

"Salmiac".

$NH_4Cl$

$NH_4Cl = 53.50$

White granular, crystalline powder or colorless crystals.

Soluble about 28% in water at room temp. About 1% in alcohol, 12% in Glycerin. It lowers the temperature of the solution when dissolving.

pH of g 5% aqueous solution is 4.5 to 6.0.

The dry material is odorless at room temperature. Strong aqueous solutions and heated crystals show odor of Ammonia.

Cool saline taste, thirst-producing.

Finds extensive use as an expectorant in prescription-free cough medicine, cough-drops, syrups, etc.

Used in licorice candy along with Anise oil or Flavor to give cool and salty taste. It will give off Ammonia odor under alkaline conditions.

Tolerated well by the human system. Pharmaceutical doses up to 3 grams per day for certain effects.

Prod. from Ammonia and Hydrochloric acid gases.

100-64;

## 115: AMMONIUM SACCHARIN

Ammonia solution. (Aqueous solution of Ammonia).
"Ammonia spirit".
Ammonia water.

$NH_3 = 17.03$ (Ammonia gas)
$NH_4OH = 35.05$ (Ammonia solution)

Colorless liquid, miscible with water.
Concentrated solution contains 27-30% $NH_3$ by weight.

Powerful and very diffusive, volatile odor. Violent chemical reaction upon mucous membranes. Lachrymator. Strong alkaline reaction. Acrid taste.

Ammonium hydroxide is probably not used "as such" in perfumery, but it does occur in small amounts in certain natural raw materials (Musk, etc.).

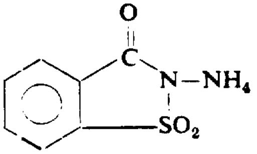
This chemical is formed during the processing of many food products, partly due to naturally occurring substances, partly due to chemicals added prior to the processing (baking powders, etc.). It is also formed when Ammonium chloride is exposed to alkaline conditions (Ammonium chloride is used in licorice flavoring).

Prod. synth. from Hydrogen plus Nitrogen.

(ref.: general commercial literature).

## 116: AMMONIUM SACCHARIN

"Sucramine".
Ammonium-*ortho*-benzsulfinimide.
"Daramin".



$C_7H_8N_2O_3S = 200.20$

White crystals or white crystalline powder. Soluble in water. Intensely sweet taste in proper dilution. Higher concentrations (in water) produce the same well-known "bitter after-taste" as Sodium saccharin.

Producers of this chemical claim that it exceeds Sodium saccharin in sweetening power. Figures as high as 700 × Sugar (cane sugar) are indicated for its effect.

Used extensively as a sweetening agent, mostly in combination with low-power sweetening chemicals, in sugar-free foods and beverages.

Aqueous solutions are very faintly alkaline.

Prod. from Saccharin.

30-331; 68-592; 100-319; 159-517;

## 117: AMMONIUM SULFIDE

NOTE: The name "Ammonium sulfide" is also (but erroneously) applied to Ammonium sulfhydrate, $NH_4HS$. That chemical is NOT described here.

$(NH_4)_2S = 68.15$

Colorless or pale yellowish liquid. Forms crystals at temperatures below 0° C.

Its strong odor is mainly due to decomposition which takes place even at room temperature. Ammonia gas, Ammonium polysulfides, Ammonium sulfhydrate, etc. are formed.

Very soluble in water, almost insoluble in alcohol and oils.

This chemical is reported used in food products at concentrations of about 5 ppm (in the finished consumer product). Mostly in spice blends. It is listed as G.R.A.S. and has F.E.M.A. No.2053.

CAUTION: Ammonium sulfide and its decomposition products yield Hydrogen sulfide gas under acid conditions. Fatal accidents have occurred when this chemical was used in cold wave hair styling.

Farmacological reports indicate that Ammonium sulfide and Ammonium sulfhydrate penetrate more rapidly through human skin than Hydrogen sulfide.

100-70; F.E.M.A.;

## 118: AMMONIUM-iso-VALERATE

Ammonium-*iso*-valerianate.
Ammonium valerate (also called, commercially).
The commercial product is the *iso*-valerate, plus *iso*-valeric acid.

Theoret. form.: $(CH_3)_2CH—CH_2—COO—NH_4$

(Theoret. Mol. wt.) $C_5H_{13}NO_2 = 119.17$

Actual formula: One Mol. Ammonium *iso*-valerate (above)
plus Two Mol. *iso*-Valeric acid, $C_5H_{10}O_2$

Total: $C_{15}H_{33}NO_6 = 323.42$

Colorless crystals, very soluble in water. Crystals become liquid in contact with moist air. Soluble in alcohol and essential oils.

It is possible to liberate the free valeric acid (*iso*-valeric acid) from the compound by diluting the saturated aqueous solution with water. The aqueous phase then contains only the Ammonium *iso*-valerate.

The compound material has a sharp, cheesy, but also somewhat sweet odor and taste. The taste is of course accompanied by acid flavor.

Used in flavor compositions for Butter, Cheese, Nut, etc. Concentrations up to 60 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2054.

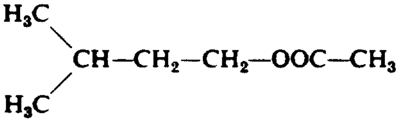
100-71;

## 119: iso-AMYL ACETATE

"Pear oil".
"Pear ether".
*iso*-Pentyl acetate.
*3*-Methyl-*1*-butylacetate (mainly).

NOTE: see also NOTE under *iso*-Amyl alcohol: There are at least two types of *iso*-Amyl acetate in the trade: One is made from fermentation Amyl alcohol (Fusel oil), the other is made from synthetic Pentanol. The two alcohols have a different composition and contain different isomers of Amyl alcohol. There are, however, flavor houses who will use the two types of Amylacetate interchangeably.

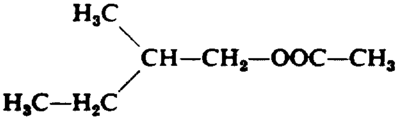
Mainly:



(up to 90% of "Fusel" Amyl acetate)

$C_7H_{14}O_2 = 130.18$

Chief second component in "Fusel" acetate: *2*-Methyl butanol-*1*-acetate = *dextro*-Amyl acetate = *secondary*-Butyl carbinyl acetate:



(from 10 to 50% of the commercial acetate)

Amyl acetate produced from synthetic Pentanol (from Pentane gas) consists mainly of *normal*-Amyl acetate:

$CH_3—(CH_2)_3—CH_2—OOC—CH_3$

*iso*-Amyl acetate is a colorless mobile liquid, B.P. approx. 142° C. Sp.Gr. approx. 0.875.

Slightly soluble (0.25%) in water, miscible with alcohol, essential oils and flavor materials.

Pronounced fruity-fresh odor, sweet but slightly nauseating. In dilution reminiscent of Pear, Banana, Apple. Very volatile.

Sweet-fruity, Pearlike, Bergamot-pear-like taste, also reminiscent of overripe Banana, Apple, etc.

Occasionally used – in mere traces – in perfumery for "lift" to heavy-oriental fragrances, florals, etc. Concentration about 0.1 to 0.2% in the perfume oil.

Used in nail polish removers and in nail polish as a solvent.

Used extensively in flavor compositions for imitation Pear, Raspberry, Strawberry, Banana, Caramel, Cola, Coconut, Apple, Cherry, Creamsoda, Grape, Butter, Peach, Pineapple, Rum, Vanilla, etc.

Concentrations up to 200 ppm in candy.

Up to 3000 ppm in chewing gum.

On account of its relatively low aroma-power, this ester often constitutes 10-20 or 40% of the entire amount of flavor ingredients in a formula.

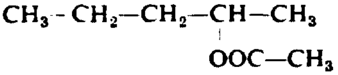
Prod.: from the alcohol (see above) by direct esterification with acetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2055.

5-236; 26-406; 33-500; 33-933; 66-586; 77-182; 23-Sept. 1948; B-II-132; 140-134; 100-569;

## 120: secondary-n-AMYL ACETATE

2-Pentanyl acetate.
*alpha*-Methyl butyl acetate.



$$CH_3-CH_2-CH_2-\underset{\underset{\displaystyle OOC-CH_3}{|}}{CH}-CH_3$$

$C_7H_{14}O_2 = 130.18$

Colorless mobile liquid. Very slightly soluble in water. miscible with alcohol and perfume or flavor materials. Sp.Gr. 0.92.
BP. = 134° C.

Powerful and diffusive, fruity, Banana-like odor, also resembling "overripe Pears".

Sweet, fruity, but not powerful taste.

Suggested for use in fruit flavors, particularly in "Tutti-Frutti" and similar combination type flavors for chewing gum, soft candy, etc.

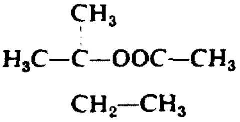
Produced directly from 2-Pentanol and Acetic anhydride – or Acetic acid under azeotropic conditions.

NOTE: Although this ester has been identified in natural fruit products, it is not yet specifically listed as G.R.A.S., and therefore not legally permitted for food use in the U.S.A.

26-406; 158-252; B-II-131;

## 121: tertiary-AMYL ACETATE

Dimethyl ethyl carbinyl acetate.
2-Methylbutanol-2-acetate.
NOTE: do not confuse with so-called "*tertiary*" -Amyl acetate, see next monograph.



$$H_3C-\overset{\overset{\displaystyle CH_3}{|}}{\underset{\underset{\displaystyle CH_2-CH_3}{}}{C}}-OOC-CH_3$$

$C_7H_{14}O_2 = 130.18$

Colorless liquid, very slightly soluble in water, miscible with alcohol and oils. B.P. 125° C. (much lower than *iso*-Amyl acetate).
Sp.Gr. 0.874.

Fresh-minty, fruity odor, not quite as sweet as the common *iso*-Amyl acetate.

Occurs in acetylated Fusel oil and is therefore a frequently appearing impurity in Amyl acetate made from Fusel oil directly.

Occasionally used in masking odors for industrial purposes.

Finds little or no use in perfumes, and is not mentioned specifically as a flavor chemical. It is reported here mainly to complete the description of various isomers of Amyl acetate.

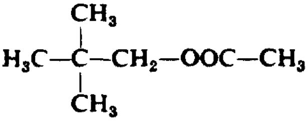
This ester has a slightly intoxicating effect upon the human CNS.

Prod. from Dimethyl ethyl carbinol by esterification with acetic acid under azeotropic conditions, or with Acetic anhydride.

26-406; 31-136; B-II-132;

## 122: »tertiary«-AMYL ACETATE

*tertiary*-Butyl carbinyl acetate.
Neo-pentyl acetate.
Trimethyl ethyl acetate.
NOTE: see preceding monograph for correct chemical name of true *tertiary*-Amyl acetate.



$$H_3C-\overset{\overset{\displaystyle CH_3}{|}}{\underset{\underset{\displaystyle CH_3}{|}}{C}}-CH_2-OOC-CH_3$$

$C_7H_{14}O_2 = 130.18$

Colorless liquid.

Fruity-fresh, somewhat green odor, reminiscent of Apples, not quite as sweet as the odor of the *iso*-Amyl acetate.

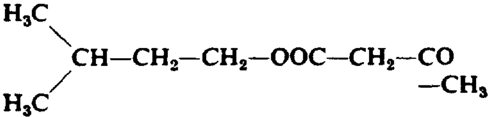
Fresh-fruity, Apple-like taste.

This ester has been suggested for use in flavors, but it has not yet been offered commercially from the usual manufacturers of perfume and flavor chemicals. To the flavorist, it may remain a curiosity, a modification of the *iso*-Amyl acetate odor/flavor.

Prod. from Trimethyl ethanol by direct esterification with acetic acid under azeotropic conditions.

31-136;

## 123: iso-AMYL ACETOACETATE



$C_9H_{16}O_3 = 172.22$

Colorless liquid, almost insoluble in water, soluble in alcohol, miscible with common flavor materials.

Ethereal-fruity, somewhat green-herbaceous, winey-sweet odor.

Fruity, green-Apple-like flavor.

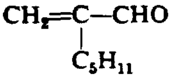
Finds some use in flavor compositions, mainly in Apple and fruity flavor types.

Concentration up to 25 ppm in the finished product (mostly candy).

G.R.A.S.

## 124: alpha-AMYL ACROLEIN

2-Octenal.
2-Pentyl acrolein.



$CH_2{=}C(C_5H_{11}){-}CHO$

$C_8H_{14}O = 126.20$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. BP. 174° C.

Peculiar green-leafy, "foliage" type odor, not as "fatty" as Octanal.

This chemical belongs to a family of many research chemicals developed in the 1930's. *beta*-Propyl acrolein, *iso*-Butyl acrolein, Hexyl acrolein, etc. are some of those which can be classified as interesting and possibly of use to the perfumer or flavorist. These unsaturated aldehydes have been identified in natural products, often used by the perfumer or flavorist.

The subject chemical finds some use in perfumery, mostly in the reconstruction of important topnotes in (artificial) essential oils.

Prod.: by condensation of Hexaldehyde with Acetaldehyde.

3-170; 89-42 (description of an isomer); 4-190; 156-26;

## 125: n-AMYL ALCOHOL

Pentyl alcohol.
*1*-Pentanol.
*n*-Butyl carbinol.

$CH_3(CH_2)_3CH_2OH$

$C_5H_{12}O = 88.15$

Colorless liquid. B.P. 138° C. Sp.Gr. 0.818.

Soluble 2.7 % in water at room temperature. Miscible with alcohol and oils.

Somewhat harsh, chemical odor, reminiscent of Fusel oil, but not as heavy, however, more penetrating, nauseating, cough-provoking. Only in high dilution fairly pleasant.

Finds occasional use in perfumery mainly for reconstruction of topnotes in (artificial) essential oils.

Used in flavor composition for imitation Berry, Apple, Banana, Chocolate, Pineapple, Rum and various types of Liqueur flavors, Brandy flavors, etc.

Concentration in finished product about 35 ppm. However, in chewing gum it may be as high as 3500 ppm.

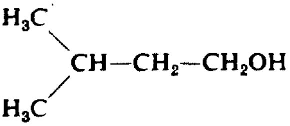
G.R.A.S. F.E.M.A. No.2056.

Prod.: (several methods) e. g. from Pentane gas (Petro-chemical).

26-406; 87-461; 100-74; B-1-383;

## 126: »iso«-AMYL ALCOHOL

"Amyl alcohol".
*iso*-Butyl carbinol.
Fusel Amyl alcohol.
Fermentation Amyl alcohol.
*iso*-Pentyl alcohol.
*3*-Methyl-*1*-Butanol.
*gamma*-Methyl-*n*-butanol.



$C_5H_{12}O = 88.15$

NOTE: The name "Amyl alcohol" and the name "*iso*-Amyl alcohol" are used in perfume and flavor trade with little respect to the identity or true chemical name of the material. Much confusion still exists, particularly since Amyl alcohol made from Fusel oil is slowly disappearing from the American market, being replaced by Amyl alcohol made from Pentane gas; this alcohol has a composition quite different from that of Fusel-Amyl alcohol.

The Fusel Amyl alcohol is the one most commonly thought of, when flavorists talk about "Amyl alcohol".

The Pentane Amyl alcohol has different impurities, specially it contains little or no *iso*-Butyl carbinol. It is mainly a *normal*-Amyl alcohol.

Colorless liquid. B.P. 132° C.
Sp. Gr. 0.813.

(these figures refer to the pure *iso*-Butyl carbinol). The boiling point is lowered by the presence of the active isomer, *secondary*-Butyl carbinol. The latter causes the commercial product to be *laevo*-rotatory. There is variable amounts from 10 to 50% of this isomer in Fermentation Amyl alcohol.

Soluble 2.7% in water at room temperature, miscible with alcohol and most perfume and flavor materials.

Choking, disagreeable, cough-provoking, somewhat alcoholic odor, only in high dilution becoming pleasant, fruity-winey.

Peculiar winey-brandy-like taste in proper dilution.

Used occasionally in perfumery, mainly in the reconstruction of essential oils (artificial ess. oils).

Used quite frequently in flavors for imitation Apple, Banana, Brandy, Chocolate, Liqueur, Rum, etc.

Concentrations up to 50 ppm in candy,
up to 100 ppm in Brandy,
up to 300 ppm in chewing gum.

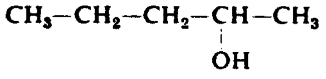
Prod. from Fusel oil (Rice, Corn, Grain, Potato, Sugar, Potato-weed, etc.). The alcohol synthesized in the Petroleum cracking industry via Pentane is a different chemical (see above notes).

G.R.A.S. F.E.M.A. No.2057.

9-17; 11-27; 26-406; 30-22; 66-311; 87-463; 100-74; B-1-392; 140-124;

## 127: secondary-n-**AMYL ALCOHOL**

*alpha*-Methyl butanol.
Methyl-*n*-propylcarbinol.
*2*-Pentanol.



$$CH_3-CH_2-CH_2-\underset{\displaystyle OH}{\underset{|}{CH}}-CH_3$$

$C_5H_{12}O = 88.15$

Colorless liquid. Sp.Gr. 0.81. BP 120°C.

Soluble 4% in water, miscible with alcohol and oils.

Winey-ethereal, rather choking odor, somewhat drier than that of commercial "Amyl alcohol".

Mainly used as an intermediate in the production of esters for fruit flavors.

Occasionally used in trace amounts in the reconstruction of certain essential oils.

Prod.:

1) by reduction of Methyl-*n*-propyl ketone.
2) from *2*-Pentene with sulfuric acid.

26-406; 66-312; 158-252; B-I-384;

## 128: iso-**AMYL AMINE**

*1-iso*-Amino pentane.
*iso*-Butyl carbylamine.

$(CH_3)_2CH-CH_2-CH_2-NH_2$

$C_5H_{13}N = 87.17$

Colorless or very pale straw-colored mobile liquid. B.P. 95° C. Sp.Gr. 0.75.

Miscible with water, alcohol, Propylene glycol, Glycerin and oils.

Unpleasant Ammonia type odor with a decay-like, "decomposition" odor.

This Amine has found some use in perfume compositions, mainly as a minute trace component in animal topnote bases, specialties, etc. It has interesting effect in Civet and Rose, blends well with Styrax and Labdanum, with Cognac oil and other ethereal-fruity and green herbal notes, etc.

The author has no record of its use in flavors.

*iso*-Amylamine is formed in Nature by decarboxylation of Leucine, e. g. by fungus action on Rye (Ergot of Rye). It is one of many common degradation products of Proteins.

Prod.:

1) from Ammonia and Amyl alcohol by heating to 350° C. over an Aluminum catalyst or Thorium oxide.
2) by reduction of *iso*-Amylnitrile (*iso*-Butyl cyanide).
3) from *iso*-Amylchloride plus Ammonia or Sodamide.

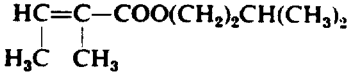
26-408; 66-398; 100-569; B-IV-180;

## 129: iso-**AMYL ANGELATE**

Angelic acid, *iso*-amylester.
*iso*-Amyl-*cis-2*-Methyl crotonate.
*iso*-Pentyl-*cis-2*-Methyl butenoate.
*iso*-Amyl-*cis-2,3*-dimethyl acrylate.

Most commercial products contain a considerable amount of the -tiglate (stereo-isomer of the -angelate).

NOTE: The literature has presented the readers with some confusion with respect to which acid is the *cis*-form and which is the *trans*-form. Above names are quoted from most recent sources.



$$\underset{H_3C}{\underset{|}{HC}}=\underset{CH_3}{\underset{|}{C}}-COO(CH_2)_2CH(CH_3)_2$$

$C_{10}H_{18}O_2 = 170.24$

Colorless liquid. B.P. 200-201° C.

Warm-herbaceous, yet refreshing-ethereal odor with winey-fruity undertones.

Herbaceous-winey taste in suitable dilution (5-20 ppm.).

Finds some use in perfumery in the reconstruction of "Roman" Chamomile oil which is very expensive and often in poor supply. Recent availability of low-cost Angelic acid has produced an increased interest in the esters.

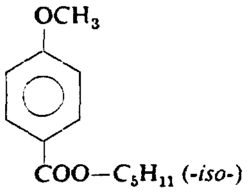
Occasionally used in flavors, mainly for liqueurs and certain types of candy, or as a trace component-modifier in minty toothpaste flavors.

Produced from Angelic acid and *iso*-Amyl alcohol by direct esterification under azeotropic conditions.

7-90; 66-311; 66-636; 90-223;

## 130: AMYL ANISATE

*iso*-Amyl anisate.
*iso*-Amyl-*para*-methoxybenzoate.



$C_{13}H_{18}O_3 = 222.29$

Colorless oily liquid. B.P. 312° C.
Sp.Gr. 1.06.

Insoluble in water, soluble in alcohol and perfume oils, poorly soluble in monoterpenes and in Propylene glycol.

Mild, sweet floral odor reminiscent of Heliotrope, fresh, soft, agreable and very tenacious.

Sweet, fruity-floral taste, however, somewhat "perfumey" in the same sense as Heliotropine.

Finds some use in perfumes as a sweetener-fixative in floral fragrances, such as Lilac, Honeysuckle, Sweet Pea, Freesia, etc. Blends well with Peru balsam, Tolu balsam, Vanillin derivatives, Anisalcohol, Heliotropine, Methoxy phenylbutanone, etc.

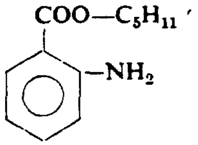
Occasionally used in flavor compositions as a modifier in Vanilla flavors, as a sweetener in fruit flavors, liqueur-flavors, etc.

Prod. by direct esterification of *iso*-Amyl alcohol with Anisic acid under azeotropic conditions.

5-350; 7-37; 28-602; 31-160; 34-680; 86-10;

## 131: AMYL ANTHRANILATE

*iso*-Amyl anthranilate.
*iso*-Pentyl-*ortho*-aminobenzoate.



$C_{12}H_{17}NO_2 = 207.28$

Colorless oily liquid. B.P. 320° C.
Sp.Gr. 1.045.

Insoluble in water, soluble in alcohol and oils, very poorly soluble in Propylene glycol.

Fruity-Plum-like, Ambre-Neroli type of odor. However, the odor type differs with the origin (manufacturer) of this chemical. Apparently, when it is chemically pure, it has very little odor. Its low odor level is improved by the addition of related, more volatile chemicals.

The taste is Plum-Grape like, quite penetrating.

Used, but rarely, in perfumes as a modifier for lower alifatic Anthranilates. It presents heavier effects, more tenacious, but less perceptible.

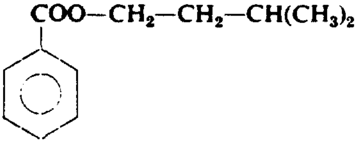
Occasionally used in flavors, for similar reasons as above, yet it seems to fortify the flavor power of the lower homologues.

Prod. by direct esterification of *iso*-Amyl alcohol with Anthranilic acid under azeotropic conditions – or: from Isatoic anhydride plus Aluminium pentoxide (amyloxide).

5-294; 31-121; 33-933; 34-1012; 102-44;

## 132: AMYL BENZOATE

*iso*-Amyl benzoate.
*3*-Methyl-*1*-butanol benzoate.
*iso*-Pentyl benzoate.



$C_{12}H_{16}O_2 = 192.25$

Colorless oily liquid. B.P. 262° C.
Sp.Gr. 0.992.

Insoluble in water, soluble in alcohol, essential oils and perfume/flavor materials.

Balsamic, mild, sweet, slightly musky Ambre-type odor. Fruity cloverlike background. Quite tenacious.

Berry- or Cherry-like flavor, faintly reminiscent also of Cocoa, Walnut or Prunes.

Finds some use in perfumery for fragrances of Oriental or Ambre-like character, in Clover ("Trefle") or "Orchid" type fragrances and as a mild fixative. It is an excellent solvent for Nitromusks, and quite stable in soap.

Used in flavor compositions for its Cherry-like, fruity notes, in imitation Apple, Bitter Almond, Cherry, Cocoa (Chocolate), Liqueurs, Hazelnut, Peach, Plum, Prune, Rum, etc.

Concentrations vary from 8 ppm in baked goods to 200 ppm in chewing gum.

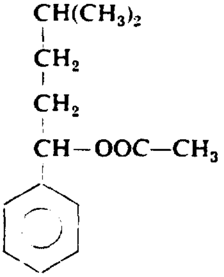
Prod. by direct esterification of *iso*-Amyl-alcohol with Benzoic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2058.

5-236; 7-38; 23- ; 27-44; 26-408; 33-933; 68-546; 86-10; 102-35; B-IX-113; 103-122; 95-184; 96-213; 140-150;

## 133: iso-AMYL BENZYL ACETATE

*alpha-iso*-Amyl phenyl carbinyl acetate.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Peculiar green-floral, sweet and somewhat herbaceous odor of good tenacity.

Finds some use in perfumery for its heavy-floral and tenacious sweetness, occasionally in Honeysuckle, Orangeblossom, Gardenia, etc.

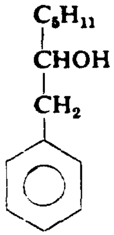
Prod. (Roure-Bertr. Fils & Justin Dupont, Grasse).

1) from *iso*-Amyl phenyl ketone (*iso*-Valerophenone) by hydrogenation followed by Acetylation.
2) from *iso*-Amyl magnesium iodide plus Benzaldehyde (Grignard reaction).

3-202; 4-68;

## 134: AMYL BENZYL CARBINOL

Benzyl amyl carbinol.
*alpha*-Amyl phenylethyl alcohol.



$C_{13}H_{20}O = 192.30$

Colorless liquid. Almost insoluble in water, soluble in alcohol and perfume oils. Poorly soluble in Propylene glycol. Sp.Gr. 0.946.

Sweet and somewhat honey-like odor of good tenacity.

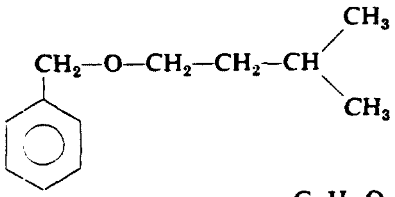
Occasionally used in perfumes for its woody-sweet, fruity-sweet or rosy-floral notes. Also as a modifier-fixative.

Prod. by Grignard synthesis, or by hydrogenation of Amyl benzyl ketone.

3-7; 5-8;

## 135: iso-AMYL BENZYL ETHER

Benzyl-*iso*-amylether.
Benzyl-*iso*-amyloxide.
*iso*-Amyl benzyl oxide.
"Gardenia oxide".
Benzyl-*iso*-pentylether.



$C_{12}H_{18}O = 178.27$

Commercial product is *iso*-Amylether, not *n*-Amylether. Colorless liquid, practically insoluble in water, soluble in alcohol and perfume materials. B.P. 235° C. Sp.Gr. 0.91.

Floral-fruity odor, somewhat greener, more herbaceous than Benzyl acetate, and much more tenacious. Overall more Gardenia-like, less Jasmin-like.

Finds some use in perfume compositions of the more heavy-floral type, such as Gardenia, Honeysuckle, Tuberose, Ylang-Ylang, and it performs excellently in soap. As an odorant, it fills the "gap" between the volatile Benzylacetate and the pungent-tenacious *para*-Cresol methylether.

The author does not know of its use in flavors.

Prod. from Benzyl chloride and *iso*-Amyl alcohol under alkaline conditions.

3-7; 5-226; 7-38; 31-147; 86-10; 102-56; 103-57; 106-74; 37-171;

## 136: AMYL BUTYRATE

Pentyl butyrate.
*n*-Amyl butyrate.
*n*-Amyl-*n*-butyrate.

NOTE: Most common commercial product is the *iso*-Amyl butyrate, see next monograph.

$CH_3{-}(CH_2)_3{-}CH_2{-}OOC{-}CH_2{-}CH_2{-}CH_3$

$C_9H_{18}O_2 = 158.24$

Colorless mobile liquid. Sp.Gr. 0.86-0.87. B.P. 186° C.

Almost insoluble in water, soluble in alcohol, essential oils, perfume and flavor materials. Insoluble in Propylene glycol and Glycerin.

Strong ethereal-fruity odor, reminiscent of Apricot, Banana, Pineapple.

Finds extensive use in flavor compositions for imitation Apple, Apricot, Banana, Butter, Butterscotch, Cherry, Fruit (Tutti-Frutti), Grape, Peach, Pineapple, Raspberry, Strawberry, Vanilla, etc.

Concentrations in finished products: up to 70 ppm.

In chewing gum as high as 800 ppm.

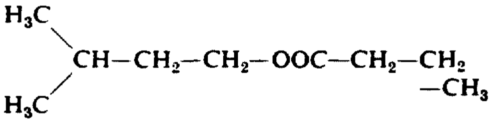
Prod. by direct esterification of *n*-Amyl alcohol with *n*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2059.

26-408; B-II-271; 100-74; 140-138;

## 137: iso-AMYL BUTYRATE

*iso*-Amyl-*n*-butyrate.
*iso*-Butyl carbinyl butyrate.
*iso*-Pentyl-*n*-butyrate.
*iso*-Pentyl-*n*-butanoate.
NOTE: This ester is commonly called "Amyl butyrate".



$C_9H_{18}O_2$ = 158.24

Colorless mobile liquid. B.P. 179° C. Sp.Gr. 0.87.

Insoluble in water, soluble in alcohol, essential oils, perfume and flavor materials.

Powerful and diffusive fruity, sweet Apricot-Banana-Pineapple-like odor, somewhat sharper than that of the *iso*-Amyl-*iso*-butyrate.

Sweet and fruity taste, not very powerful, yet stronger than the acetate.

Extensively used in flavor compositions. This ester may constitute a large percentage of many fruit flavors, such as: imitation Apricot, Banana, Cherry, Peach, Strawberry, "Tutti-frutti", etc. and in Butter, Butterscotch, Chocolate, etc.

Concentration in finished product may be 80 ppm in candy, and up to 550 ppm in chewing gum.

Occasionally used to impart "lift" to perfumes and to modify "creamy" notes with Amyl phenylacetate, Vanillin, etc.

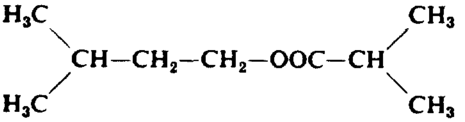
Prod. by direct esterification of *iso*-Amyl alcohol with *n*-butyric acid under azeotropic conditions. If Fusel-Amyl alcohol is used, the resulting ester has a slightly different aroma.

G.R.A.S. F.E.M.A. No.2060.

FCC 1964-781; B-II-171; 5-236; 7-38; 23- ; 31-136; 26-408; 86-11; 102-35; 106-48; 128-25; 95-181; 140-138;

## 138: iso-AMYL-iso-BUTYRATE

*iso*-Butyl carbinyl-*iso*-butyrate.
*iso*-Pentyl-*iso*-butyrate.
NOTE: This ester is often called: Amyl-*iso*-butyrate.



$C_9H_{18}O_2$ = 158.24

Colorless mobile liquid. B.P. 169° C. Sp.Gr. 0.88.

Insoluble in water, miscible with alcohol, soluble in essential oils, perfume and flavor materials.

Fruity-Apricot-Pineapple type odor, softer and sweeter than that of the *iso*-Amyl-*n*-butyrate.

Sweet fruity taste, suggestive of Apricot, Peach, Pineapple and other fruits.

Finds limited use in perfumery as a modifier for Amyl phenylacetate and other heavy esters, or as a trace component topnote item.

Extensively used in flavor compositions for introduction of light, fruity notes: Apple, Apricot, Banana, Berry, Peach, etc.

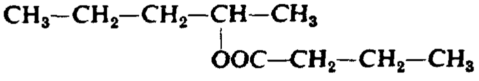
Concentration in finished consumer product: up to 70 ppm in candy, and up to 2000 ppm in chewing gum.

Prod. from *iso*-Amyl alcohol and *iso*-Butyric acid by direct esterification under azeotropic conditions.

33-732; 26-408; B-II-291; 77-185;

## 139: secondary-n-AMYL BUTYRATE

*alpha*-Methyl butyl butyrate.
Methyl-*n*-Propyl-carbinyl butyrate.
*2*-Pentyl butyrate.



$$CH_3{-}CH_2{-}CH_2{-}\underset{\displaystyle OOC{-}CH_2{-}CH_2{-}CH_3}{\underset{|}{CH}}{-}CH_3$$

$C_9H_{18}O_2 = 158.24$

Colorless liquid.

Fruity, heavy-sweet, diffusive odor, reminiscent of Banana and Peach.

Sweet, heavy-fruity taste, not very powerful, mainly of the Peach type, more Apricot-like in highly acid media.

Suggested for use in fruit flavors of the "Tutti-Frutti" type, particularly in chewing gum, where diffusive power is desirable.

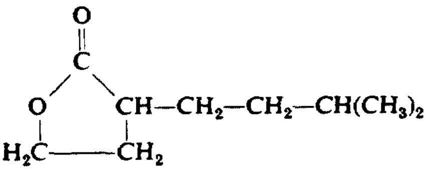
NOTE: This ester is NOT specifically listed as G.R.A.S. in the U.S.A.Federal Register.

Prod.: by direct esterification of *2*-Pentanol with *n*-Butyric acid under azeotropic conditions.

158-252;

## 140: alpha-iso-AMYL-gamma-n-BUTYROLACTONE

*iso*-Nonanolide.
NOTE: This is the *alpha*-substituted isomer of the well-known Nonanolide (so-called Aldehyde C-18) also known as *gamma*-Nonalactone, see Nonanolide-*1,4*.



$C_9H_{16}O_2 = 156.23$

Colorless oily liquid. Insoluble in water, soluble in alcohol, essential oils, perfume and flavor materials. Poorly soluble in Propylene glycol and mineral oil.

Musky, Ambregris-like odor with an oily-fatty note. The main difference between this lactone and the *gamma*-isomer seems to be the lack of nutlike notes in the former, the muskiness and overall drier character.

This lactone, only rarely offered commercially, has found some use in flavor compositions and little – if any – in perfumes. It does not seem to offer enough of interesting or unusual notes that it can become a permanent item on the perfumer's or flavorist's shelf.

Prod.: from Ethylene oxide by *iso*-Amyl malonic ester synthesis.

31-170; 156-229;

## 141: AMYL CAPRATE

*iso*-Pentyl decylate.
*iso*-Pentyl decanoate.
*iso*-Amyl caprinate.

$(CH_3)_2CH{-}CH_2{-}CH_2{-}OCC(CH_2)_8CH_3$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid. B.P. 282° C.
Sp.Gr. 0.86

Insoluble in water, soluble in alcohol and essential oils, poorly soluble in Propylene glycol.

Oily-winey, brandy-like odor with mild fruity undertones.

Brandy-Rum-like taste in extreme dilution, otherwise fatty-oily, also reminiscent of Hazelnut and Coconut.

Finds some use in perfumery in substitutes for natural Cognac oil.

This ester finds some use in flavor compositions for imitation Apple, Arak, Brandy, Rum, Quince, Pear, etc., usually applied in mere traces. Accompanied by esters of lower alifatic acids, it lends richness and power to these as an interesting modifier.

Prod. by direct esterification of *iso*-Amyl alcohol with Decanoic acid under azeotropic conditions.

4-8; 77-187; 140-143;

## 142: AMYL CAPROATE

Pentyl hexanoate.
*n*-Amyl-*n*-hexylate.

$CH_3(CH_2)_3CH_2$—OOC—$(CH_2)_4CH_3$

$C_{11}H_{22}O_2 = 186.29$

Colorless liquid. B.P. 226° C. Sp.Gr. 0.861.

Insoluble in water, soluble in alcohol, essential oils, perfume and flavor materials.

Pungent-fruity, yet refreshing odor, reminiscent of Pineapple, Apple, and remotely of Pear.

Pineapple-like taste, sweet-sharp fruity, powerful, somewhat green-fruity undertone.

Probably not used in perfumes.

Finds use in flavor compositions for imitation Apple, Chocolate, Citrus, Grape, Honey, Liqueur-types, Pineapple, etc.

Concentration usually up to 50 ppm in the finished product. In chewing gum as high as 110 ppm.

G.R.A.S. F.E.M.A. No.2074.

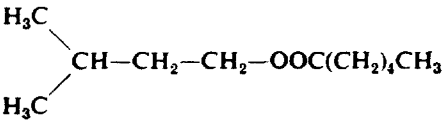
Prod.: by azeotropic esterification of *n*-Amylalcohol with *n*-Hexanoic acid.

26-408; 44-1230; B-II-323; 140-141;

## 143: iso-AMYL CAPROATE

"Amyl hexylate" (Fusel-Amyl caproate).
*iso*-Pentyl-*n*-hexanoate.
*iso*-Amyl-*n*-hexoate.

NOTE: this ester is commercially known as: Amyl caproate (incorrect). It is occasionally offered under name of "Pineapple aldehyde" probably confused with Allyl caproate.



$$(H_3C)_2CH-CH_2-CH_2-OOC(CH_2)_4CH_3$$

$C_{11}H_{22}O_2 = 186.29$

Colorless liquid. Sp.Gr. 0.865. B.P. 222° C.

Insoluble in water, soluble in alcohol, essential oils, perfume and flavor materials.

Somewhat sharp, Apple-Banana-Pineapple-like odor.

Fresh-fruity, Apple-Pineapple type flavor.

Probably not used in perfumery.

Frequently used in flavor compositions for imitation Apple, Honey, Raspberry, Rum, Pineapple, Strawberry, etc.

Concentrations up to 16 ppm in finished product.

Prod. by direct esterification of the *iso*-Amyl alcohol with Caproic (=Hexanoic) acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2075.

4-8; 26-408; 77-186; 90-212; 140-141;

## 144: AMYL CAPRYLATE

Amyl octanoate.
Pentyl octoate.

$CH_3(CH_2)_3CH_2{-}OOC(CH_2)_6CH_3$

$C_{13}H_{26}O_2 = 214.34$

Colorless liquid. Sp.Gr. 0.85. B.P. 260° C.

Insoluble in water, soluble in alcohol, essential oils, perfume and flavor materials.

Sweet-oily, fruity odor with distinct "perfumey" floralness: Orris-Elderflower notes, under a Banana-like topnote.

Finds some use in perfumery, but is rarely preferred over Hexyl caprylate, more popular for this purpose: a modifier in Oriental fragrances, a companion to Ionones, a modifier-fixative in topnotes for Oriental fragrances, etc.

Finds some use in flavor compositions for imitation Chocolate, Fruit (tutti-frutti, etc.), Liqueur and Brandy flavors, etc.

Concentrations are usually little more than traces, up to 7 ppm in the finished product.

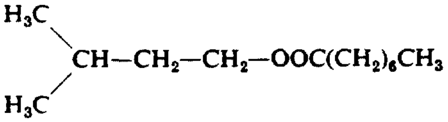
G.R.A.S. F.E.M.A. No.2079.

Prod. by direct esterification of *n*-Amyl alcohol with Caprylic acid under azeotropic conditions.

26-408; 103-121;

## 145: iso-AMYL CAPRYLATE

*iso*-Amyl octanoate.
*iso*-Pentyl octylate.
*iso*-Amyl-*n*-caprylate.
Note: This ester is often marketed under the name: Amyl caprylate.



$C_{13}H_{26}O = 214.34$

Colorless liquid. Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol, perfume and flavor materials.

Peculiar oily-fruity, slightly animal odor reminiscent of Elderflower, with orris undertones.

The author does not know of its use in perfumery.

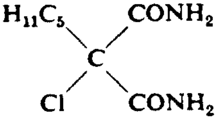
Used in flavor compositions for imitation Chocolate, Fruit (mostly the heavier types), Liqueur and Brandy flavoring, etc.

Concentrations are usually traces (a few ppm) up to 7 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2080.

Produced by direct esterification of the *iso*-Amyl alcohol with Octanoic acid (*n*-Caprylic acid) under azeotropic conditions.

## 146: n-AMYL CHLOROMALONAMIDE



$C_8H_{15}ClN_2O_2 = 206.68$

White powder. Soluble in water, somewhat soluble in alcohol.

Practically odorless.

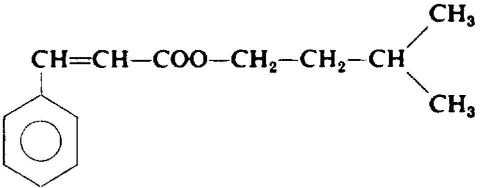
Intensely sweet taste. Estimated sweetness: 400 times that of cane sugar in aqueous solution.

The author knows of no commercial use of this chemical in foods. It seems to have exclusively academic interest because the *iso*-Amyl chloromalonamide is not sweet, but rather bitter of taste.

30-321; 159-505;

## 147: iso-AMYL CINNAMATE

"Amyl cinnamate" (commercial name).
*iso*-Amyl-*beta*-phenylacrylate.
*iso*-Pentyl cinnamate.
*iso*-Pentyl-*beta*-phenylacrylate.
*iso*-Pentyl-*3*-phenylpropenoate.



$C_{14}H_{18}O_2 = 218.30$

Colorless, somewhat viscous liquid. Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol. B.P. 310° C. Sp.Gr. 1.00.

Faintly balsamic, mild Ambre-like, Cocoa-bean-like (fresh beans), with undertones of Orchid-Labdanum, slightly animal and very tenacious odor.

Sweet and heavy flavor, somewhat reminiscent of Cocoa, also floral and "perfumey", Ambre-like.

Used in perfumes for Oriental notes, Chypre, Ambre, and as a fixative-blender in spicy fragrance types (Carnation etc.). Quite stable in soap and a fair fixative. However, it tends to polymerize in storage. An increasing cloudiness, accompanied by increased viscosity and decreased odor level are signs of beginning polymerization.

Used in flavors for imitation Butter, Caramel, Fruit, Honey, Peach, Pineapple, Strawberry, etc. and in traces in Vanilla compositions to introduce warm-balsamic notes resembling Cocoa or Chocolate.

Concentrations in finished foods: up to 12 ppm in candy or baked goods.

G.R.A.S. F.E.M.A. No.2063

E.O.A. No.264.

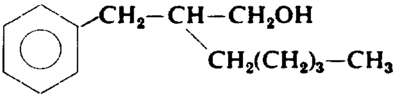
Prod. by direct esterification of *iso*-Amyl alcohol with Cinnamic acid (commercial *trans*-Cinnamic acid) under azeotropic conditions.

4-9; 5-236; 5-269; 7-38; 23; 24; 34-933; 28-603; 35-462; 35-463; 86-11; 102-35; 103-122; 128-27;

## 148: AMYLCINNAMIC ALCOHOL

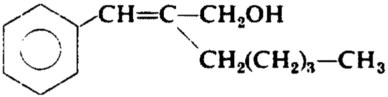
*alpha*-Pentyl cinnamyl alcohol.
Buxinol.
Amyl cinnamyl alcohol.
*alpha-n*-Amyl cinnamyl alcohol.

NOTE: Certain commercial products are contaminated with substantial amounts of Amyl dihydrocinnamyl alcohol (also called *2*-Benzyl-*1*-heptanol):



$C_{14}H_{22} = 206.32$

Amyl dihydro cinnamyl alcohol.
Less desirable odor.



$C_{14}H_{20}O = 204.31$

Amyl cinnamic alcohol.
Desirable, floral odor.

AMYL CINNAMIC ALCOHOL:
Colorless or almost colorless oily liquid. Insoluble in water, soluble in alcohol and oils. Very mild, oily-waxy-floral, sweet and pleasant, tenacious odor.

Used in perfumes as a modifier for the aldehyde in floral fragrances. Introduces natural notes, but is very weak, unless accompanied by more volatile components of related odor type.

Oxidizes under exposure to air and may produce undesirable, fatty or "aldehydic" notes.

Used in trace amounts in chocolate flavor compositions.

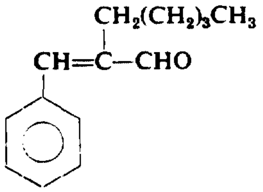
Prod. from Amyl cinnamic aldehyde by heating with Benzyl alcohol in presence of NaOH. More commonly by Ponndorf reaction from Amyl cinnamic aldehyde.

G.R.A.S. F.E.M.A. No.2065.

156-29; 4-11; 4-27; 155-88;

## 149: AMYL CINNAMIC ALDEHYDE

Flosal (Descollonges).
Buxine (Givaudan).
Mahonia (Firmenich).
Jasmonal.
Floxine.
Flomine.
Jasmylal.
Jasminyl.
Jasmin aldehyde.
*alpha-n*-Amyl cinnamic aldehyde.
Amyl cinnamal.
*alpha*-Pentyl-*beta*-phenyl acrolein.
"A.C.A.".
Heptyllis.
*2*-Benzylidene-heptanal.



$C_{14}H_{18}O = 202.30$

Pale yellowish oily liquid. Sp.Gr. 0.96-0.97. B.P. approx. 285° C.

Very mild oily-herbaceous and somewhat floral odor, reminiscent of many types of natural flowers, but mostly of Jasmin, Gardenia and Tuberose.

Soluble in alcohol and perfume materials. Insoluble in water.

Used very extensively in perfumes, including soap perfumes. Introduces Jasmin-like floralness when accompanied by more volatile chemicals of floral character. Blends excellently and assists in fixation of the fragrance (ACA is quite tenacious). There is a marked difference in odor quality and floral effect between "high-grade" Amyl cinnamic aldehyde and "regular" or commercial (prime, etc.) grade. Lots from various producers also show considerable difference in odor quality. ACA is very susceptible to oxidation unless properly treated with an antioxidant (conventionally added by most manufacturers). Old or oxidized ACA has objectionable, rancid-fatty odor. Lower grades of ACA may show by-odor of Benzaldehyde, Heptaldehyde or Amyl nonenal, sometimes called Di-heptenal.

Concentration in perfumes may vary from 2 to 10%, in exceptional cases up to 30-35%.

Used in flavor compositions for imitation Apple, Apricot, Peach, Spice, Strawberry, Walnut, usually in traces only.

In chewing gum the concentration may reach 15 ppm.

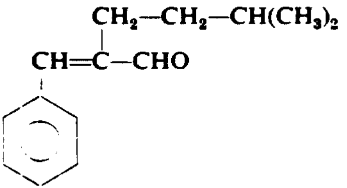
Prod. from Heptanal (from cracked Castor oil) by condensation with Benzaldehyde in alkaline solution. The vacuumdistilled product is stabilized with 0.15 to 0.5% Diphenylamine as an antioxidant.

G.R.A.S. F.E.M.A. No.2061.

4-11; 5-142; 26-410; 68-986; 86-12; 103-255; 154-783; 155-88; 156-27; B-VII-310;

## 150: alpha-iso-**AMYLCINNAMIC ALDEHYDE**

*iso*-Amylcinnamal.



$C_{14}H_{18}O = 202.30$

Viscous yellowish oil. B.P. 261° C.
Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol, miscible with oils, poorly soluble in Propylene glycol.

Warm-oily, herbaceous odor, less floral, but warmer than *n*-Amylcinnamic aldehyde. Its lower boiling point results in a poorer tenacity and a somewhat less delicate initial note.

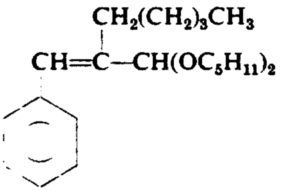
This aldehyde has been produced and offered commercially, but apparently without any success. Most observers agree that it does not offer any noticeable advantages over the conventional *n*-Amylcinnamic aldehyde, which is produced on a very large scale and available at a very low cost.

Prod.: from *iso*-Amyl acetaldehyde and Benzaldehyde in a Claisen condensation.

93-150;

## 151: alpha-**AMYLCINNAMIC ALDEHYDE-DI-AMYLACETAL**

NOTE: the *iso*-Amyl acetal is included in this description.



$C_{24}H_{40}O_2 = 360.58$

Colorless or very pale yellowish liquid.

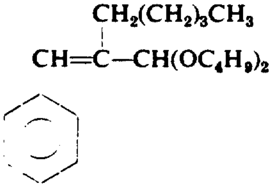
Practically odorless when pure, but may introduce mild-herbaceous, oily-green and slightly vinous notes when used as a modifier of the Aldehyde or its lower Acetals.

Not regularly offered as a commercially available chemical.

Prod. from Amylcinnamic aldehyde and (*iso*-)Amyl alcohol.

156-27;

## 152: alpha-**AMYLCINNAMIC ALDEHYDE-DI-BUTYL ACETAL**



$C_{22}H_{36}O_2 = 332.53$

Colorless or very pale yellowish liquid.

Faint and rather nondescript odor, somewhat herbaceous and oily-green, overall nonfloral. Apparently weak, but quite tenacious.

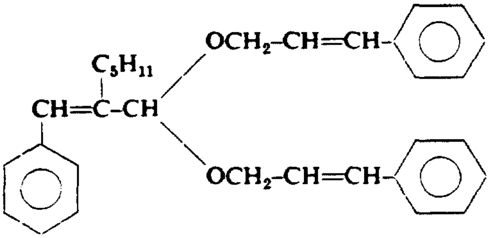
Not generally offered as a commercially available chemical.

This Acetal can find some use in perfume formulations as a modifier for lower Acetals, and as an olfactory stabilizer due to its considerable tenacity. However, it does not seem to contribute any interesting notes to the odor picture of related chemicals.

Produced from Amylcinnamic aldehyde and Butylalcohol.

156-27;

## 153: AMYL CINNAMIC ALDEHYDE DICINNAMYL ACETAL



$C_{32}H_{36}O_2 = 452.64$

Almost colorless, oily liquid. Sp.Gr. 1.01. BP. 222° C.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and perfume oils.

This acetal is described as having a Caraway-type odor, but the author does not quite agree, since he finds only a very mild, warm-herbaceous, almost floral-green odor with a trace of spicy undertones. However, this description is based upon the evalutation of one single sample of subject material.

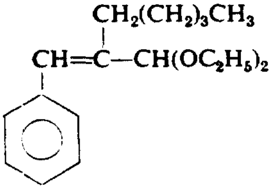
The author would assume that this Acetal has little or no interest to the creative perfumer. It does not offer any unusual notes or power, and its main virtue could only be that of a high-cost fixative.

Prod.: from Amylcinnamic aldehyde and Cinnamic alcohol by condensation.

37-512;

## 154: AMYLCINNAMIC ALDEHYDE DIETHYL ACETAL

*1,1*-Diethoxy-*2*-amyl-*3*-phenyl-*2*-propene.
*alpha-n*-Amylcinnamal diethylacetal.



$C_{18}H_{28}O_2 = 276.42$

Almost colorless oily liquid. Pale yellowish color usually indicate a content of free aldehyde (ACA).

Practically insoluble in water. Soluble in alcohol and perfume materials. Poorly soluble in Propylene glycol.

Faintly oily, green-leafy and simultaneously floral odor, reminiscent of the herbal-floral part of Jasmin. Good tenacity.

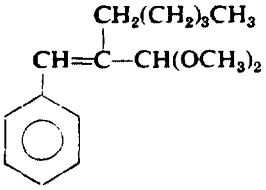
This chemical is unstable under acid conditions (certain flavor uses).

Prod. from Amylcinnamic aldehyde and Ethyl alcohol by condensation.

86-12; 103-284; 156-27;

## 155: AMYLCINNAMIC ALDEHYDE DIMETHYL ACETAL

*alpha-n*-Amylcinnamal dimethylacetal.
*1,1*-Dimethoxy-*2*-amyl-*3*-phenyl-*2*-propene.



$C_{16}H_{24}O_2 = 248.37$

Almost colorless slightly oily liquid. A yellowish tint or color usually indicates a significant content of the free aldehyde (ACA).
Sp.Gr. 0.94. B.P. approx. 300° C.

Almost insoluble in water, soluble in alcohol and perfume materials.

Peculiar animal-green odor, mild and reminiscent of parts of the Jasmin complex, although not very floral unless composed with related Jasmin chemicals. The odor is strongly influenced by the presence of even minute amounts of free aldehyde.

Used quite frequently in perfume compositions as a modifier-blender for Amylcinnamic aldehyde and a fixative for the more volatile portion of the Jasmin complex (Benzyl acetate, etc.). Excellent as a modifier in general in floral compositions, to introduce naturalness and "petal-like" notes.

Used as a trace component in certain types of flavor compositions. Yet, it should be noted that this chemical is NOT stable under aqueous acid conditions (many flavors are used in such media).

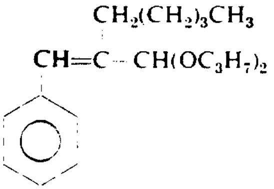
Prod. from Amylcinnamic aldehyde and Methyl alcohol by condensation.

G.R.A.S. F.E.M.A. No.2062.

5-321; 43-158; 38-I-604; 84-2; 4-11; 106-51; 103-284; 86-13; 156-27;

## 156: alpha-**AMYLCINNAMIC ALDEHYDE-DI**-(iso)-**PROPYL ACETAL**

Note: this monograph includes the *iso*-propyl acetal.



$C_{20}H_{32}O_2 = 304.48$

Almost colorless oily liquid.

Oily-herbaceous, somewhat green-balsamic odor, not very characteristic of any natural material.

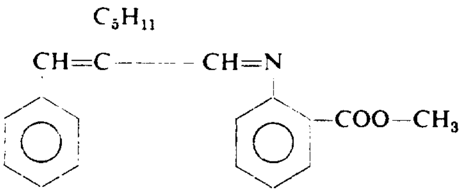
This Acetal is not generally offered as a commercially available chemical, but it finds occasionally use in perfume compositions as a modifier for lower Acetals, and as a mildly odorous fixative in Jasmin, Tuberose and other heavy-floral fragrance types.

Prod. from Amylcinnamic aldehyde and Propylalcohol (or *iso*-Propyl alcohol) by condensation.

156-27;

## 157: alpha-**AMYLCINNAMIC ALDEHYDE-METHYLANTHRANILATE**

A "Schiff's Base".
"Jasmalique" (Fritzsche Bros. Co.).



$C_{22}H_{25}NO_2 = 335.45$

Yellow viscous liquid. Insoluble in water, soluble in alcohol and perfume materials, poorly soluble in Propylene glycol.

Sweet-floral, predominantly Orangeblossom-like odor with oily-herbaceous undertones, reminiscent of Honeysuckle, Gardenia, Tuberose, remotely of Jasmin and other heavy florals.

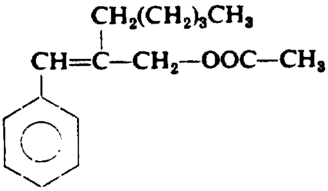
Used mainly for its highly fixative purposes. Its tenacity being one of its greatest assets, this material can be incorporated in numerous types of floral fragrances, the concentration varying from less than one percent to several percent in Orangeblossom or Honeysuckle types.

Prod. by condensation of Amylcinnamic aldehyde with Methyl anthranilate to form the conventional Schiff's base. The purity of the components and the stoechiometric calculation of the two components, the process of condensation, etc., all have considerable influence upon the odor type of the outcoming base.

(Fritzsche Bros. sample).

## 158: AMYL CINNAMYL ACETATE

*alpha*-Pentyl cinnamyl acetate.
*alpha-n*-Amyl-*beta*-phenylacryl acetate.
Floxin acetate.



$C_{16}H_{22}O_2 = 246.35$

Sp.Gr. (higher than 1.0). Colorless oily liquid. Soluble in alcohol and oils.

Mild oily-fruity and somewhat green odor with balsamic and faintly floral undertones.

Finds but little use in perfumery, mainly as a modifier for floral-green components of Jasmin and other floral complexes.

Occasionally used in flavor compositions, for imitation Chocolate, Fruit and Honey flavors – usually in traces only.

NOTE: This ester is not very stable under acid-aqueous conditions (a condition often encountered in functional products with artificial flavor).

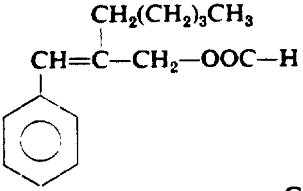
Prod. from Amylcinnamic alcohol and Acetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2064.

4-11;

## 159: AMYL CINNAMYL FORMATE

*alpha*-Pentyl cinnamyl formate.
*alpha-n*-Amyl-*beta*-phenylacryl formate.
Floxin formate.



$C_{15}H_{20}O_2 = 232.33$

Colorless liquid.

Oily-herbaceous, sweet and slightly green-balsamic odor with some resemblance to Butter-caramel.

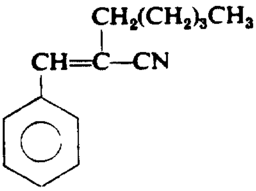
The author does not know of its use in perfumes.

Used occasionally in flavors for imitation Chocolate, Fruit, Maple, Nut, etc., usually in mere traces.

G.R.A.S. F.E.M.A. No.2066.

## 160: alpha-AMYL CINNAMYL NITRILE

*alpha*-Amyl-*alpha*-cyanostyrene.



$C_{14}H_{17}N = 199.30$

Colorless liquid.

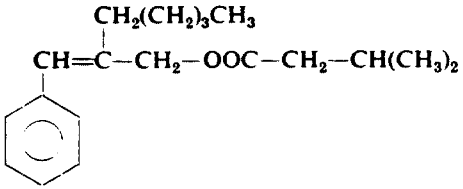
Peculiar herbaceous-green, somewhat earthy-nutlike odor. Sharper than Amyl cinnamic aldehyde, but bears some resemblance to that.

Developed as a member of a series of Nitriles in research for the purpose of substituting less stable aldehydes with the corresponding nitrile. In many cases, the nitrile has an odor very similar to that of the aldehyde (Benzonitrile-Benzaldehyde, Geranylnitrile – Citral, etc.).

This nitrile has – to the author's knowledge – not found wide use in perfumery or flavor work.

## 161: AMYL CINNAMYL-iso-VALERATE

*alpha*-Pentyl cinnamyl-*iso*-valerate.
*alpha-n*-Amyl-*beta*-phenylacryl-*iso*-valerate.
Floxin-*iso*-valerate.



$C_{19}H_{28}O_2 = 288.43$

Colorless liquid.

Mild fruity, somewhat herbaceous-tobacco-like odor.

Fruity-oily, warm and slightly spicy-tobaccolike, haylike flavor.

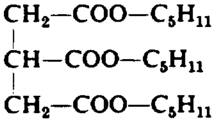
Occasionally used in flavor compositions for imitation Chocolate, Fruit, Grape and Nut flavors, usually in mere traces.

Prod. from Amylcinnamic alcohol and *iso*-Valeric acid by direct esterification under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2067.

## 162: AMYL CITRATE

Triamyl citrate.



$$\begin{array}{l} CH_2-COO-C_5H_{11} \\ | \\ CH-COO-C_5H_{11} \\ | \\ CH_2-COO-C_5H_{11} \end{array}$$

$C_{21}H_{38}O_6 = 386.54$

Colorless liquid. B.P. (higher than 300° C.).

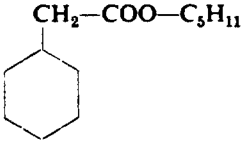
Very faint odor, vinous-herbaceous type.

Occasionally used as a solvent for perfume or flavor materials, but not as commonly as Triethyl citrate.

Its very high boiling point (and low vapour pressure) makes it useful as a fixative-blender-diluent for industrial perfumes.

## 163: AMYL CYCLOHEXANE ACETATE

Cyclohexane acetic acid, Amylester.
Amyl hexahydrophenylacetate.



$C_{13}H_{24}O_2 = 212.34$

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful, sweet and fruity odor of moderate tenacity. The fruity notes are rather nondescript, or they may be classified as remotely resembling Raspberry-Banana type.

This ester has been suggested for use in flavors, but it appears that this and many related esters are not widely used for such purpose, one of the reasons probably being the regrettable confusion surrounding the description and nomenclature of these chemicals.

See notes under monograph: Ethyl cyclohexane acetate.

Until these materials are clearly defined and officially declared permissible in food flavors, it would be safe to concentrate on perfume experiments with these materials.

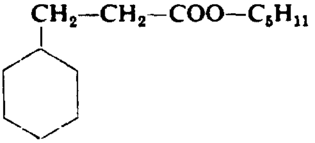
The title ester could introduce very pleasant nuances in lipstick perfumes, and its power and fruity character would make it suitable for perfumes in functional products including a masking problem (hairsprays, hair setting lotions, shampoos, etc.). Powerful fruity chemicals are often successful in overcoming or eliminating sulfuraceous odors, amine-odors, etc. from cosmetic ingredients.

Prod.: by esterification of Amylalcohol with Cyclohexane acetic acid.

140-144;

## 164: AMYL CYCLOHEXANE PROPIONATE

Cyclohexane propionic acid, Amylester.
Amyl hexahydrophenyl propionate.



$C_{14}H_{26}O_2 = 226.36$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity odor of Banana-Pineapple-Pear type, but far from being a "natural" odor. Moderate to good tenacity. Sweet fruity taste in concentrations well below 10 ppm, perceptible (by most observers) at concentrations below 1 ppm.

This ester has been suggested for use in flavor compositions, but it is not specifically mentioned in the American Federal Register, nor is it deemed G.R.A.S. by the F.E.M.A. in the U.S.A. However, it is most conceivable that the material is used in flavors outside the United States of America.

Much confusion surrounds the naming and identification of these esters. The reader is encouraged to read the note on that subject under monograph: Ethyl cyclohexane acetate.

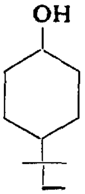
The title ester could find good use in perfume compositions for its power and masking ability towards sulfuraceous and proteinic odors, often encountered in modern cosmetic preparations.

Prod.: by direct esterification of Amylalcohol with Cyclohexane propionic acid, using azeotropic conditions.

140-144;

## 165: para-tertiary-AMYL CYCLOHEXANOL

"Methyl Patchone".
"Homo Patchone".



$C_{11}H_{22}O = 170.30$

White crystals. Sublimes when heated.

Insoluble in water, soluble in aqueous alkali, in alcohol and oils.

Dry, pine-woody odor of good tenacity, yet of considerable diffusive power.

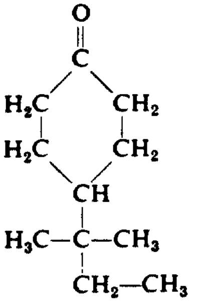
Although very much of the same odor characteristics as the popular "Patchone" (*para-tertiary*-Butyl cyclohexanol), this higher homologue has not achieved the same popularity. It has less of the Patchoulicharacter, is even drier and not quite as powerful.

It blends well with the Ionones, with other Cyclohexyl derivatives, Amylsalicylate, *iso*-Bornylacetate and other Pine needle odors, etc.

Prod.: by hydrogenation of *para-tertiary*-Amylcyclohexanone, also known under the trade name "Orivone".

## 166: para-tertiary-AMYL CYCLOHEXANONE

Orivone (I.F. & F.).
Irinone (Maywood).



$C_{11}H_{20}O = 168.28$

Colorless liquid. Insoluble in water, soluble in alcohol and perfume materials.

Very powerful, diffusive, woody-camphoraceous odor, slightly earthy, yet with some resemblance to Orris root, overall very dry.

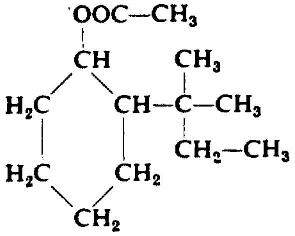
Finds extensive use in perfumery, at low concentration, for its power, soap stability and compatibility with Ionones, Lavandin oil, etc.

Prod. from *para-tertiary*-Amyl cyclohexanol with $CrO_3$-oxidation, (from *para-tertiary*-Amyl phenol by hydrogenation).

(IFF publ. in Chem Week, 1961).

## 167: ortho-tertiary-AMYL CYCLOHEXYL ACETATE

Coniferan (I.F.F.).



$C_{13}H_{24}O_2 = 212.34$

Colorless liquid, soluble in alcohol, essential oils and perfume materials.

Camphoraceous, balsamic-green and somewhat sweet odor, reminiscent of certain Pine needle oils, and with good tenacity. Its woody undertones makes it compatible with Patchouli oil, making the overall odor drier.

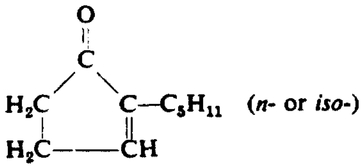
Used in perfumery not only for Pine fragrances, but generally as a modfier for numerous other derivatives of Cyclohexanol. Stable in alkali under normal conditions. For woody, powdery, herbaceous-camphoraceous fragrance types.

Prod. from *ortho-tertiary*-Amyl cyclohexanol, which in turn is produced from the corresponding phenol, by hydrogenation.

(I.F.F.).

## 168: AMYL CYCLOPENTENONE

See Note below.
*2-n*-Amyl cyclopenten-*2*-one-*1*.
"Nor-*iso*-jasmone".



$C_{10}H_{16}O = 152.24$

Colorless or very pale straw-colored liquid. Insoluble in water, soluble in alcohol, miscible with perfume oils.

Fruity, fresh-floral and Jasmin-like odor, but it lacks the "bread-like" note of the Jasmine, a note found in *cis*-Jasmone and in the Methyl jasmonates. The odor of Amyl cyclopentenone is not as rich as the odor of the named materials.

Suggested for use in perfume compositions, primarily in the creation of artificial Jasmin, Jasmin bases, specialties, etc. It can also be used as a floralizer for fragrances other than those of the Jasmin type, mainly in the milder florals, and in a few sharper ones, such as Hyacinth.

NOTE: Most literature sources claim that the *iso*-Amyl cyclopentenone has a preferable odor with respect to Jasmine similarity. It is most conceivable that some of the "Amyl cyclopentenones" commercially available are actually *iso*-Amyl cyclopentenone.

Prod.: from Decenoic acid by treatment with Phosphoric acid.

156-222; (sample: Compagnie Parento, Inc.).

## 169: AMYL ETHER

*iso*-Amyl ether (commercial product is *iso-)*.
Di-*iso*-amylether.
*iso*-Pentylether.
*iso*-Amyl oxide.

$$\left[(CH_3)_2CH(CH_2)_2\right]_2O$$

$$C_{10}H_{22}O = 158.29$$

– including various isomers.

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 173° C. Sp.Gr. 0.78 (*n*-Amyl ether: 190° C. and 0.77).

Peculiar faint odor, yet choking-nauseating when concentrated. Ethereal without being winey, green but not natural. Has a slightly metallic undertone. In dilution remotely reminiscent of Pear.

Finds occasionally use in perfumery, mostly in industrial odors where its powerful masking effect towards certain solvent odors can be utilized.

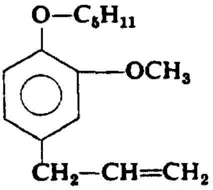
Probably not used in flavors.

Prod.:
1) from *iso*-Amylalcohol by dehydration.
2) from *iso*-Amylbromide and Sodium amylalcoholate.

B-I-401; 31-144; 66-324; 26-478; 86-42; 1-120; 4-8; 37-176;
see also: 100-75.
The Di-*n*-amylether is rarely, if ever, used in perfumes or flavors.

## 170: AMYL EUGENOL

"Amyl-oxy-eugenol".
Eugenol amylether.
*1*-Pentoxy-*2*-methoxy-*4*-allylbenzene.



$$C_{15}H_{22}O_2 = 234.34$$

Pale yellowish, viscous liquid.

Insoluble in water, soluble in alcohol and perfume oils, poorly soluble in Propylene glycol.

Sweet-spicy, somewhat herbaceous-floral, heavy odor of considerable tenacity. Overall drier than the Amyl-*iso*-eugenol, and not nearly as interesting or versatile to the perfumer/flavorist.

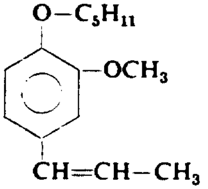
Useful as a modifier in Carnation fragrances, in heavy florals, Ylang Ylang compositions, Honeysuckle, Tuberose, Narcisse, etc.

Occasionally used in flavor compositions for Vanilla, Chocolate, Cream-caramel, etc., but is generally inferior to the Amyl-*iso*-eugenol in this respect.

Prod. from Eugenol in alcoholic Potassium hydroxide solution with Amyl bromide.

## 171: AMYL-iso-EUGENOL

*iso*-Eugenol amylether.
Amyl oxy-*iso*-eugenol (P & S old name).
*1*-Pentoxy-*2*-methoxy-*4*-propenylbenzene.
Exists as *cis*- or *trans*-isomer, the latter being predominant in the commercial product.



$C_{15}H_{22}O_2 = 234.34$

Pale yellowish, very viscous liquid. Insoluble in water, soluble in alcohol, perfume and flavor materials, poorly soluble in Propylene glycol.

Sp.Gr. 1.04. B.P. approx. 300° C.

Heavy-sweet, balsamic-floral and very faintly spicy odor of exceptional tenacity.

Useful in perfumes as a modifier for other *iso*-Eugenol derivatives, in Carnation, Tuberose, Narcisse, Ylang-Ylang, Champaca, certain types of Rose and many other florals. It will also act as a fixative blender, and performs very well with Patchouli, Vetiver, Oakmoss and other Chypre materials.

Finds some use in flavor compositions for imitation Chocolate (Cocoa), Vanilla, Butterscotch, Caramel, etc.

Prod. from *iso*-Eugenol in alcoholic Potassium hydroxide solution with Amyl bromide, or by isomerization of Amyl eugenol.

4-10; 155-88;

## 172: AMYL FORMATE

*n*-Pentyl formate.

$CH_3(CH_2)_3CH_2$—OOC—H

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.90.
B.P. 132° C.

Very slightly soluble in water. Miscible with alcohol, perfume and flavor materials.

Powerful ethereal-vinous, somewhat dry-earthy, yet fruity odor with earthy-green undertones.

Sweet- fruity, vinous and fresh taste.

Finds use in flavor compositions for imitation Apple, Apricot, Banana, Cherry, Blackcurrant, Nut, Rum, Peach, Plum, Strawberry, Walnut flavors, etc.

Concentrations in finished consumer product: up to 30 ppm. Concentrations in chewing gum may be as high as 150-170 ppm.

Prod. from Amyl alcohol and Formic acid by direct esterification under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2068.

26-410; B-II-22;

## 173: iso-AMYL FORMATE

*iso*-Pentyl formate.
NOTE: commercial "Amyl formate" is often *iso*-Amyl formate.

$(CH_3)_2CH$—$CH_2$—$CH_2$—OOC—H

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 124° C.

0.3% soluble in water, miscible with alcohol, perfume and flavor materials, almost insoluble in Glycerin.

Peculiar green-fruity, deep-sweet odor, almost nauseating undertone. Ethereal-volatile (diffusive) apple-winey topnote. Resembles also Blackcurrant and Plum.

Pleasant sweet-fruity, winey taste, mostly apple-like.

Has found a little use in perfumery for its peculiar leather-like topnote effect. This ester is unstable in alkali.

Frequently used in flavor compositions, primarily in imitation Apple. Also for: Apricot, Banana, Blackcurrant, Cherry, Peach, Pineapple, Plum, Strawberry, etc.

Concentrations in finished product: up to 30 ppm. – except in chewing gum: up to 250 ppm.

Prod. by direct esterification of *iso*-Amyl alcohol with Formic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2069.

FCC-1964-785.

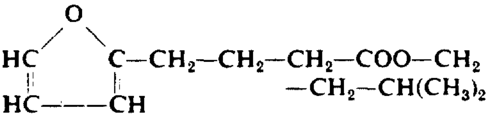
4-9; 5-235; 26-410; 77-179; 86-11; 103-84; 106-52; 128-29; B-II-22;

NOTE: The ester presents a certain degree of fire hazard (flash point 42° C.).

## 174: iso-**AMYL-2-FURANBUTYRATE**

*2*-Furanbutyric acid, *iso*-amylester.
*iso*-Pentyl-*2*-furanbutyrate.
*alpha*-*iso*-Amyl furfuryl propionate.
Amyl furfhydracrylate (old name).

NOTE: Do not confuse this chemical with: Amyl furan propionate (next).



$C_{13}H_{20}O_3 = 224.30$

Pale yellowish liquid.

Sweet-buttery, fruity and caramel-like odor, rather heavy, but also natural and pleasant in high dilution.

Used in flavor compositions for imitation Chocolate, Coffee, Fruit (tutti-frutti), Whisky & Brandy, etc.

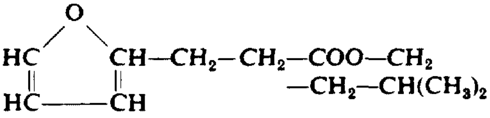
Concentration in finished product: up to 8 ppm.

Prod. from Furfural.

G.R.A.S. F.E.M.A. No.2070.

## 175: iso-**AMYL-2-FURAN PROPIONATE**

*iso*-Amyl furfuryl propionate.
*iso*-Pentyl-*2*-furanpropionate.
*alpha*-*iso*-Amyl furfurylacetate.
*iso*-Amyl furfurhydracrylate.
*2*-Furanpropionic acid, *iso*-amylester.



$C_{12}H_{18}O_3 = 210.27$

Colorless liquid, but may turn pale yellowish under storage. Insoluble in water, miscible with alcohol, perfume and flavor materials.

Sweet-green, somewhat floral odor with a distinctly fruity note, sweet-caramellic undertone.

Rarely used in perfumery, probably as a trace component in Violet type fragrances or as a modifier-topnote material for fruity-green topnotes in "modern" fragrances.

Used in flavor compositions for imitation Chocolate, Coffee, Tutti-frutti, Whisky/Brandy, etc.

Concentration is usually mere traces (a few ppm. in finished product).

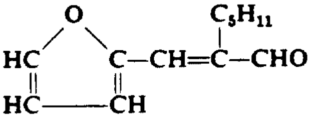
Prod. from Furfurhydracrylic acid with *iso*-Amyl alcohol by direct esterification. The acid is obtained by hydrogenation of *2*-Furanacrylic acid, which in turn is prepared from Furfural plus Malonic acid with Pyridine as a catalyst. Furfural is a common commercial chemical obtained by destructive oxidation of waste carbohydrates.

G.R.A.S. F.E.M.A. No.2071.

77-197;

## **176:** alpha-**AMYL FURFURACROLEIN**

*alpha*-Amyl furylacrolein.
*alpha*-Furfurylidene heptanol.
*alpha*-Amyl-*beta*-*2*-furylacraldehyde.



$C_{12}H_{16}O_2 = 192.24$

Yellow liquid. Soluble in alcohol and perfume oils. B.P. 256° C. Sp.Gr. 1.00.

Sweet-herbaceous, floral, somewhat spicy-Ambre-like odor of good tenacity.

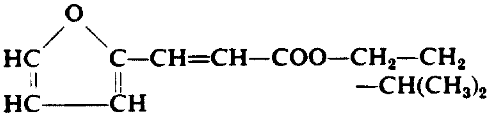
This chemical has found little use in perfumery, but it forms membership of a series of *alpha*-alkyl-substituted Furfuracroleins of which the lower members are very interesting to the Aroma industries, mainly for flavor purposes.

Prod. from Furfural and Heptaldehyde, by condensation.

31-38; 31-40; 69-154; 93-150;

## **177:** iso-**AMYL FURFURYL ACRYLATE**

"*iso*-Amyl furylacrylate".
*iso*-Amyl-*beta*-furylacrylate.
*iso*-Amyl-*2*-furancrotonate.



$C_{12}H_{16}O_3 = 208.25$

Colorless or pale yellowish liquid.
Sp.Gr. 1.03. B.P. approx. 250° C.

Insoluble in water, miscible with alcohol, perfume and flavor materials.

Heavy, pungent, sweet-fruity odor, reminiscent of Pineapple, Rum, fruit preserves, wine, etc. with a herbaceous-floral undertone.

Sweet-fruity, pineapple-like taste.

Occasionally used in perfumes.

Has been used in flavor compositions for imitation Pineapple, Rum, etc. – but:

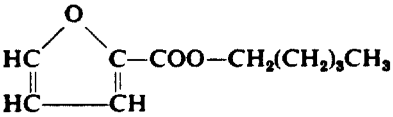
NOTE: This material is no longer approved for use in food flavorings in the U.S.A. (Dec. 1964).

Prod. from *2*-Furanacrylic acid and *iso*-Amylalcohol. The acid is produced from Furfural and Malonic acid with Pyridine catalyst.

86-11; 26-410;

## **178: AMYL FUROATE**

Amyl pyromucate.
Pentyl-*2*-furoate.
*2*-Furoic acid, *n*-amylester.
Furan-*alpha*-carboxylic acid, *n*-amylester.
Pyromucic acid, *n*-amylester.



$C_{10}H_{14}O_3 = 182.24$

Colorless or very pale yellowish liquid.

Almost insoluble in water, soluble in alcohol, perfume and flavor materials.

Sweet-caramellic-winey, "fermented" odor.

This ester finds use in flavor compositions for imitation Rum, Maple, Caramel, Butterscotch, etc.

Concentration in finished product usually about 10 ppm.

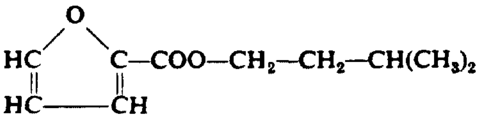
Prod. by direct esterification of Pyromucic acid with Amyl alcohol. The acid is prepared from Furfural by oxidation.

G.R.A.S. F.E.M.A. No.2072.

69-157 (homologues); 140-174;

## 179: iso-AMYL FUROATE

*iso*-Pentyl furan-*alpha*-carboxylate.
*iso*-Amyl pyromucate.
*iso*-Amyl-*2*-furoate.



$C_{10}H_{14}O_3 = 182.24$

Colorless liquid. B.P. approx. 230° C.

Insoluble in water, soluble in alcohol and oils.

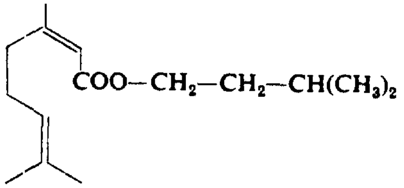
Sweet-fruity, caramellic and somewhat floral odor.

Occasionally used in flavor compositions (NOTE: the *iso*-Amylester is not specifically included in the G.R.A.S. list in the U.S.A.).

Prod. (analogous to the Amyl furoate).

26-410; 140-174;

## 180: iso-AMYL GERANATE



$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

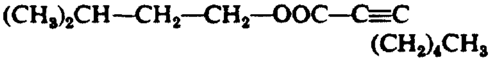
Mild, herbaceous-winey, remotely floral odor of moderate tenacity.

This ester is used, but very rarely, in perfume compositions, partly as component of artificial essential oils, partly as a novel note in perfumes of non-floral character, modern Chypres, etc.

Prod.: by direct esterification of Geranic acid with *iso*-Amylalcohol, preferably under azeotropic conditions.

## 181: iso-AMYL HEPTIN CARBONATE

"Vert de Violette".
*iso*-Amyl octynoate.
*iso*-Amyl heptin carboxylate.



$$(CH_3)_2CH{-}CH_2{-}CH_2{-}OOC{-}C{\equiv}C\,(CH_2)_4CH_3$$

$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid. B.P.approx. 250° C. Sp.Gr. 0.915.

Insoluble in water, soluble in alcohol and oils.

Powerful, but also sweet-leafy-green odor, closely resembling the odor of crushed Violet leaves. Less pungent, and less fatty than the lower alkyl heptin carbonates.

This ester, known for over 60 years, was considerered the ideal Violet-leaf odor until the appearance of Nonadienal and Nonadienol in the mid-1920's.

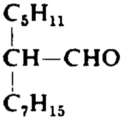
Still used in perfumery as a specific topnote ingredient in many floral fragrances – other than Violet: Lilac, Sweet Pea, Tuberose, Gardenia, etc.

Prod. from Heptyne-sodium and *iso*-Amyl chloroformate. Heptyne is usually prepared from Heptaldehyde, which is derived from Castor oil.

4-9; 5-245; 103-295; 155-86; 156-11;

## 182: AMYL HEPTYL ACETALDEHYDE

"Di-heptanal".
"Di-oenanthal".
"Aldehyde *iso*-C-14".
Note: Do not confuse with Di-heptenal (see below).



$$\begin{array}{l} C_5H_{11} \\ \vert \\ CH{-}CHO \\ \vert \\ C_7H_{15} \end{array}$$

$C_{14}H_{28}O = 212.36$

Colorless waxy solid mass, melting at 30° C. to a colorless oily liquid. Sp.Gr. 0.83.
B.P. 268° C.

Insoluble in water, soluble in alcohol and oils.

Mild citrusy-waxy odor with a faintly fruity note reminiscent of Banana pulp (the non-ethereal note) or Peach (the dry note).

Has been suggested for use in perfume compositions, and may find some use in artificial flower absolutes and aldehydic topnote compositions, as a modifier/fixative. However, its low odor level makes it rather uninteresting as an active ingredient.

Prod.:

1) By condensation of 2 Mol. Heptanal, followed by hydrogenation.
2) The above condensation product, *n*-Amylnonenal, is a by-product in the manufacture of Amylcinnamic aldehyde, and the unsaturated Amyl-nonenal can be hydrogenated to the title material.

36-1029;

## 183: AMYL HEPTYLATE

Amyl heptanoate.
Pentyl heptoate.
"Amyl oenanthate".

$CH_3(CH_2)_3CH_2{-}OOC(CH_2)_5CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Insoluble in water, soluble in alcohol, perfume and flavor materials.

Peculiar oily-green, dry-fruity odor.

Occasionally used in flavor compositions for imitation Coconut, Fruit (tutti-frutti), Lemon, Nut, etc.

Concentration in finished products up to 8 ppm.

In chewing gum as high as 50 ppm.

Produced by direct esterification of Amyl alcohol with Heptanoic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2073.

## 184: iso-AMYL HEPTYLATE

*iso*-Pentyl heptoate.
*iso*-Amyl-*n*-heptanoate.

$(CH_3)_2CH{-}CH_2{-}CH_2{-}OOC{-}C_6H_{13}$

$C_{12}H_{24}O_2 = 200.32$

Colorless mobile oil. Sp.Gr. 0.866.

Insoluble in water, soluble in alcohol, perfume and flavor materials.

Peculiar green-fruity, somewhat grassy odor, reminiscent of Bananas and unripe fruits.

Occasionally used in flavor compositions for imitation Coconut, Banana, Apple, Nut, etc.

Prod. by direct esterification of *iso*-Amyl alcohol with *n*-Heptanoic acid under azeotropic conditions.

4-9; 17-39; 43-933; 45-61; 86-11; 103-121;

## 185: iso-AMYL HEPTYL ETHER

*n*-Heptyl-*iso*-amylether.
Amyl heptyl ether (commercial name often applied).
*iso*-Amyl heptyl oxide.

$(CH_3)_2CH—CH_2—CH_2—O—CH_2(CH_2)_5—CH_3$

$C_{12}H_{26}O = 186.34$

Colorless liquid. Sp.Gr. 0.795.
B.P. approx. 210° C.

Almost insoluble in water, soluble in alcohol and perfume materials.

Oily-green, herbal odor, reminiscent of fresh-cut flowers stems, rather bitter-green, but refreshing and natural.

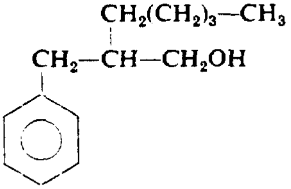
This ether finds some use in perfumery as a modifier for the more violent green smelling chemicals. It is much less pungent than most of the conventional "green" materials, but it is also rather "specific" in its odor type, therefore not as versatile in use.

Prod. from *iso*-Amyl alcohol and Heptanol by dehydration (in liquid form or in vapor form).

4-69; (see also: 30-240; 31-344;)

## 186: alpha-AMYL HYDROCINNAMIC ALCOHOL

Dihydro amylcinnamic alcohol.
*alpha-n*-Amyl phenyl propanol.
*alpha-n*-Pentyl phenyl propyl alcohol.



$C_{14}H_{22}O = 206.33$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and perfume materials. B.P. approx. 270° C. Sp.Gr. 0.943.

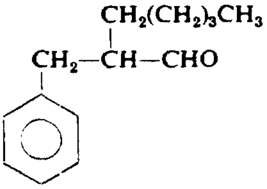
Mild, faint, oily-herbaceous odor, sweet and tenacious, like green wood.
Used occasionally in perfume compositions of Jasmin, Reseda, Hyacinth type, Oriental types, and in general as a blender for Amyl cinnamic aldehyde, Cinnamic alcohol, Phenyl propyl alcohol, etc. as well as in fancy woody compositions ("Mahogany" etc.).

Prod. by hydrogenation of Amyl cinnamic alcohol.

3-10; 86-11; 155-98; 93-152;

## 187: alpha-AMYL HYDROCINNAMIC ALDEHYDE

*alpha*-Amyl phenylpropionic aldehyde.
*alpha-n*-Amyl phenyl propyl aldehyde.
Dihydro amylcinnamal.



$C_{14}H_{20}O = 204.32$

Colorless oily liquid. Sp.Gr. 0.93.

Almost insoluble in water, soluble in alcohol and perfume materials. Faint, oily-floral, also somewhat herbaceous-green odor, overall very mild and bearing some similarity to the odor of Amylcinnamic aldehyde diethylacetal.

Useful as a modifier for Amylcinnamic aldehyde in herbaceous-floral fragrance complexes, and generally as a blender-modifier, mainly in Jasmin, Lilac, Muguet and similar fragrance types.

It does not have the power of Amylcinnamic aldehyde, and the material is really of little more than academic interest.

Prod.:

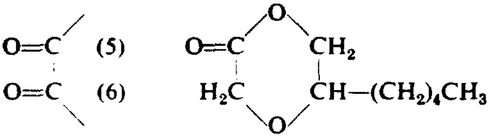
1) from Amylcinnamic alcohol via Amylhydrocinnamic alcohol by oxidation to the title aldehyde.
2) by selective hydrogenation of Amylcinnamic aldehyde.

See also: Amylcinnamic alcohol.

3-10; 155-98;

## 188: 2-AMYL-5-KETO-1,4-DIOXAN

Commercial product may be:
*2*-AMYL-*6*-KETO-*1*,*4*-DIOXAN



(5-KETO-)

$C_9H_{16}O_3 = 172.22$

Colorless liquid. Almost insoluble in water.

Fruity-winey, somewhat ethereal odor with caramellic undertone.

Used in flavor compositions as a trace ingredient and partly as a fixative in fruity-winey-caramellic flavor types. These flavors are often applied to baked goods, candy, Icecream, etc.

Concentration is usually not higher than 5 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2076.

(see also: 69-1529).

## 189: iso-AMYL KETONE

Di-*iso*-amylketone.
*iso*-Caprone.
*2*,*8*-Dimethyl-nonan-*5*-one.

$[(CH_3)CH(CH_2)_2]_2{-}CO$

$C_{11}H_{22}O = 170.29$

Colorless or pale yellowish oily liquid.
B.P. 226° C.

Insoluble in water, soluble in alcohol and oils.

Rather sharp, fatty-fruity and sweet odor, reminiscent of Apricot and Orange.

Fruity-fatty taste.

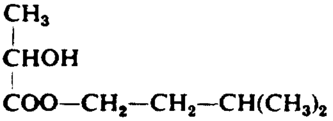
Used occasionally in flavor compositions for imitation Apricot, Peach, Plum, etc.

Prod. - usually by the "ketonic fission" method from the corresponding *beta*-keto acid ester, or: from *iso*-Caprone-dicarboxylic acid with dilute sulfuric acid.

4-69; 26-478; 66-509; 66-517; B-I-714; 86-42;

## 190: AMYL LACTATE

*iso*-Pentyl-*beta*-hydroxy propionate.
(Commercial material is usually *iso*-).



$$\begin{array}{l} CH_3 \\ | \\ CHOH \\ | \\ COO{-}CH_2{-}CH_2{-}CH(CH_3)_2 \end{array}$$

$C_8H_{16}O_3 = 160.22$

Colorless oily liquid. B.P. 210° C.
Sp.Gr. 0.971.

Very slightly soluble in water, soluble in perfume materials, flavor materials and alcohol. Fairly soluble in Propylene glycol.

Very mild oily-winey odor. To some people virtually odorless.

Has been used in certain flavor compositions as a solvent and modifier for Ethyl lactate, Ethyl butyryl lactate, etc. in imitation Butter, Milk, Cream and similar flavors. It remains, however, a comparatively rare and uninteresting chemical.

Produced from Lactic acid and *iso*-Amyl alcohol by direct esterification under azeotropic conditions.

4-9; 26-410; B-III-265; 158-186;

## 191: iso-AMYL LAURATE

*iso*-Amyl dodecylate.
Amyl laurate (commercial name).
*iso*-Pentyl dodecanoate.

$(CH_3)_2CH—CH_2—CH_2—OOC—(CH_2)_{10}CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid. Insoluble in water, soluble in alcohol and perfume and flavor materials.

Occasionally used as a fixative, more often as a solvent in perfume compositions. It has excellent properties as a solvent for Resins, Resinoids, Gums, Oleoresins, etc., and for poorly soluble crystalline perfume materials (Nitromusks, etc.).

Its odor is extremely faint, oily-fatty, dependent upon the quality of the parent Lauric acid.

The ester is occasionally used in flavor compositions, mainly for special effects (fatty-fruity notes) in Peach and similar flavors.

It is also used generally in fruit flavor compositions and for liqueur flavorings.

Concentration in finished product up to 7 ppm.

G.R.A.S. F.E.M.A. No.2077.

Prod.: by direct esterification.

3-8; 4-9; 86-12; 103-216; 155-86;

## 192: iso-AMYL LEVULINATE

*iso*-Amyl laevulate.
*iso*-Amyl acetopropionate.
*iso*-Amyl-*gamma*-ketovalerate.

$(CH_3)_2CH—CH_2—CH_2—OOC—CH_2—CH_2—CO—CH_3$

$C_{10}H_{18}O_3 = 186.25$

Colorless oily liquid. B.P. 242° C.
Sp.Gr. 0.96.

Almost insoluble in water, soluble in alcohol and oils.

Warm, winey-caramellic odor of good tenacity.

Mild, oily-caramellic and slightly fruity taste.

Although this ester appears to be very suitable for flavor compositions, it is not listed in the American G.R.A.S. list or permitted by the Federal Register.

But it does find some use in perfume compositions for its "natural" and "rounding-off" effect upon herbaceous compositions. It has very pleasant effects with Clary Sage, Lavender, Coriander, etc., and it will take the harshness out of Amylsalicylate, Coumarin, etc. for sweet-herbaceous and winey odor types.

The ester has excellent effect in imitation Rum, Butter, Caramel, Apple "Champagne", etc. and the author believes that it is used outside of the U.S.A.for flavor compositions.

Prod.: by direct esterification of *iso*-Amylalcohol with Levulinic acid, preferably under azeotropic conditions.

B-III-207, dritter Ergänzbd.

## 193: AMYL MALONATE

Diamyl malonate.
Diamyl methane dicarboxylate.

$COO-C_5H_{11}$

$CH_2$

$COO-C_5H_{11}$

$C_{13}H_{24}O_4 = 244.34$

Colorless oily liquid. Sp.Gr. 0.963.

Insoluble in water, soluble in alcohol and perfume materials.

Mild, fruity odor with a somewhat green-herbaceous undertone.

Fruity, but also somewhat bitter and not particularly pleasant taste.

This ester could find some use in perfumery as a modifier for fruity (volatile) notes, partly as a fixative for such notes.

The ester would not be of interest to the flavor industry.

Prod. from Malonic acid and Amylalcohol by direct esterification under azeotropic conditions.

4-9; 30-313;

## 194: AMYL MERCAPTAN

"Pentalarm".
(This commercial product is a mixture of isomer Amylmercaptans).
*l*-Pentanethiol.
Amyl thioalcohol.

$C_5H_{11}SH$

$C_5H_{12}S = 104.21$

Colorless mobile liquid. B.P. 126° C. Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol, perfume and flavor materials.

Extremely penetrating, unpleasant odor, typical of the mercaptans, sulfuraceous, choking, gassy.

This mercaptan is used as a "tracer" in household and industrial gas at a concentration low enough to make the odor of the gas bearable, but high enough to warn the user, that the otherwise odorless gas is present at a hazardous concentration. Methane, Propane and Butane industrial gases can be almost odorless and would present explosion and fire hazards if not properly "marked" by this warning mercaptan.

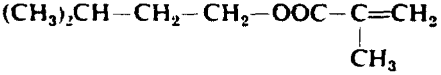
Apart from its original use in academic study of the relationship between the human olfactory perception and the Raman shift of various odorous substances, this mercaptan has probably found very little use in perfume or flavor compositions.

Prod. from Amylbromide and Potassium sulfhydrate in cold alcoholic solution.

100-75; 30-263; 30-264; 86-12; 1-121; 159-34; 159-559; 159-578;

## 195: iso-AMYL METHACRYLATE

*iso*-Amyl-*alpha*-methylacrylate.



$(CH_3)_2CH-CH_2-CH_2-OOC-\underset{\displaystyle CH_3}{\underset{|}{C}}=CH_2$

$C_9H_{16}O_2 = 156.21$

Colorless mobile liquid. Insoluble in water, soluble in alcohol, perfume and flavor materials. Poorly soluble in Propylene glycol.

Powerful ethereal, pungent, fruity-apple-like very diffusive odor. Somewhat choking, remotely reminiscent of Pineapple.

Since the acid and several esters of 2-Methacrylic acid have been identified in essential oils, fruits, etc. it has been suggested that this ester could be used in flavors.

In most countries, however, it remains to be proven that these esters are harmless at ordinary use concentrations. before it could be recommended that they are included in flavor compositions.

Methacrylic esters are comparatively unstable when exposed to air unless properly stabilized with inhibitors. Most esters are supplied with inhibitor already added. Polymerization leads to increased viscosity and decreased odor in the product.

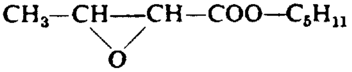
These chemicals are manufactured by the large chemical producers of plastics and plexiglas, not by the perfume or flavor houses.

Produced by ester exchange reaction.

(see also 90-116;)

## 196: AMYL METHYL GLYCIDATE

Commercial product is *beta*--Methyl amyl glycidate:
Amyl-*alpha-beta*-epoxy-*beta*-methylacetate.
*beta*-Methyl-*alpha-beta*-epoxyacetic acid, Amylester.



$CH_3{-}CH{-}CH{-}COO{-}C_5H_{11}$ (epoxide O bridging the two CH)

$C_9H_{16}O_3 = 172.21$

Colorless oily liquid. Very slightly soluble in water, soluble in alcohol, perfume and flavor materials.

Fruity, somewhat green, but also sweet and tenacious odor, remotely reminiscent of Strawberry, with a "cooked" note, almost caramellic.

This ester has been suggested for use in imitation fruit flavors, but it is not listed as being officially used in the U.S.A.

## 197: AMYL MYRISTATE

*iso*-Amyl myristate.
*iso*-Pentyl tetradecanoate.

$C_5H_{11}{-}OOC(CH_2)_{12}CH_3$

$C_{19}H_{38}O_2 = 298.51$

Colorless oily liquid. B.P. 320° C.
Sp.Gr. 0.865.

Very mild, waxy odor, to some persons it is absolutely odorless.

Has occasionally been used as a blender/modifier in fragrances of Violet type, or other fragrances where Ionones play an important role. It may contribute a faint "petal-like" effect in floral fragrances, but is generally considered too weak to produce a reasonable odor value.

Prod. from *iso*-Amyl alcohol and Myristic acid.

86-12;

## 198: iso-AMYL NITRATE

Amyl nitrate (often called).

$(CH_3)_2CH{-}CH_2{-}CH_2{-}ONO_2$

$C_5H_{11}NO_3 = 133.15$

Colorless mobile liquid. Sp.Gr. 0.996.
B.P. 147° C.

Insoluble in water, soluble in alcohol and oils.

Ethereal-fruity, vinous odor with a peculiar musty undertone, rather typical of many alkyl nitrates.

Sweet taste in high dilution.

Has been used in pharmaceutical preparations, but is probably not used any longer in perfume or flavor industries. Occasional reports seem to indicate that this ester could introduce an "aged" note in alcohol for perfume and cologne use, but the author has doubts that this application is in practise.

Prod. from *iso*-Amyl alcohol and Nitric acid in the presence of urea to control the formation of $HNO_2$.

4-9; 26-472; B-I-403; 66-335;

## 199: iso-AMYL NITRITE

"Amyl nitrite" (often called).

$(CH_3)_2CH—CH_2—CH_2—O—NO$

$C_5H_{11}NO_2 = 117.15$

Pale yellowish mobile liquid. Sp.Gr. 0.88. B.P. 99° C.

Slightly soluble in water, miscible with alcohol and oils.

Extremely diffusive, ethereal-fruity, penetrating odor.

Sweet taste in high dilution.

Decomposes in air and daylight.

Beyond its use – still in force – as a powerful vasodilator of quick, short action, this ester is probably not used in perfumes or flavors.

It presents a considerable hazard in that its vapors form explosive mixtures with air, and its relatively measurable toxicity should ban it from experimental use in foods or cosmetics.

Prod. from *iso*-Amyl alcohol, Sodium nitrite, water and diluted Sulfuric acid.

1-113; 26-410; 66-336; 85-27; 100-75; B-I-402;

## 200: iso-AMYL NONYLATE

*iso*-Amyl pelargonate.
*iso*-Pentyl nonanoate.
*iso*-Amyl nonanoate.
Nonate.

$(CH_3)_2CH—CH_2—CH_2—OOC(CH_2)_7CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid. B.P. 260-265° C. Sp.Gr. 0.86.

Somewhat nutty-oily, fruity-vinous, Apricot-like odor with a faint floral background, remotely rosy.

Probably not used to any great extent in perfumery, but finds use in flavor compositions for fruit types, imitation Cognac, Rum, etc.

Concentrations are usually as low as 4 ppm in the finished product.

Prod. from *iso*-Amyl alcohol and Pelargonic (Nonanoic) acid by direct esterification under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2078.

4-10; 86-12; 103-121; 140-143;

## 201: iso-AMYL OCTIN CARBONATE

*iso*-Amyl-*n*-oct-*1*-yne-carboxylate.
*iso*-Pentyl nonynoate.

$(CH_3)_2CH—CH_2—CH_2—OOC—C\equiv C(CH_2)_5CH_3$

$C_{14}H_{24}O_2 = 224.35$

Colorless liquid. B.P. approximately 260° C. Sp.Gr. 0.90.

Powerful green foliage odor, less pungent and less sharp than the Methyl heptin carbonate, and not as fatty, overall more "oily", yet pleasant.

Finds some use in perfumery, although always in extremely low concentration, as a modifier for lower alkyl heptin or alkyl octin carbonates, not only for Violet fragrances, but also for other florals, such as Narcisse, Tuberose, Gardenia, etc.

Prod. from Octyne via Octyne sodium with *iso*-Amyl chloroformate to form the ester.

4-9; 86-12; 155-86; 156-11;

## 202: AMYL OLEATE

*iso*-Amyl oleate.

$C_5H_{11}—OOC—C_7H_{14}—CH{=}CH—C_8H_{17}$

$C_{23}H_{44}O_2 = 352.58$

Colorless or pale yellowish oily liquid.
Sp.Gr. 0.897. B.P. approximately 340° C.

Insoluble in water, soluble in alcohol and most perfume materials, but almost insoluble in terpenes and other hydrocarbons.

Very faint "oily" odor, varying with the quality and age of the material.

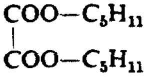
Has been suggested for use in perfumery to introduce "fatty" or "oily" notes in substitute bases for flower absolutes, etc.

Prod. from Oleic acid (Elain) and *iso*-Amyl alcohol.

4-9; 26-410; B-II-467;

## 203: AMYL OXALATE

Diamyl oxalate.



$$\begin{array}{l} COO—C_5H_{11} \\ | \\ COO—C_5H_{11} \end{array}$$

$C_{12}H_{22}O_4 = 230.31$

Colorless liquid. B.P. approximately 265° C.
Sp.Gr. 0.97.

- Virtually odorless when pure, this ester may have a trace of an odor, depending upon its quality.

It has been suggested for use as a solvent in perfume compositions but does not seem to offer advantages over the newer and more conventional solvents.

Prod. from Amyl alcohol and Oxalic acid.

4-9; 86-12;

## 204: iso-AMYL-n-PENTIN CARBONATE

*iso*-Amyl hexynoate.
*iso*-Amyl-*n*-pent-*1*-yne carboxylate.

$(CH_3)_2CH—CH_2—CH_2—OOC—C{\equiv}C(CH_2)_2CH_3$

$C_{11}H_{18}O_2 = 170.17$

Colorless liquid. B.P. approximately 220° C.

Sharp and pungent green foliage type odor, almost choking-gassy in the pure state, more pleasant at concentrations below 0.1% in an odorless solvent.

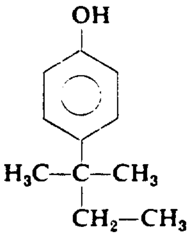
Has been suggested for use in perfume compositions as a modifier for Methyl heptin carbonate and other alkyl pentin, hexin, heptin or octin carbonates. It is slightly more floral than MHC but almost as pungent.

Prod. from Methyl propyl ketone to make *n*-Pent-*1*-yne. Pentyne sodium is reacted with *iso*-Amyl chloroformate to yield the ester.

5-245;

## 205: para-tertiary-AMYL PHENOL

Pentaphen.
Amyl phenol.



$C_{11}H_{16}O = 164.25$

Crystal needles. M.P. 93° C. B.P. 267° C.

Very slightly soluble in water, soluble in alcohol, essential oils and most perfume chemicals.

Very dry "phenolic" – medicinal odor, sometimes described as "leatherlike", but more appropriately "tanning-odor".

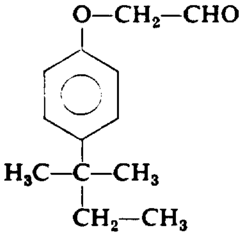
Occasionally used in perfumery for "Russian Leather" effects (Cuir de Russie) or as a modifier for rectified Birch Tar oil which is a scarce and poorly available material.

Its odor is reduced considerably under alkaline conditions, and it produces discoloration in presence of minute amounts of Iron.

Prod.: (several methods) e. g. *tertiary*-Amyl alcohol plus Phenol in presence of Aluminium chloride. Also by olefinic alkylation.

26-410; 68-423; 100-76; B-VI-548;

## 206: para-tertiary-AMYL PHENOXY ACETALDEHYDE



$C_{13}H_{18}O_2 = 206.19$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Heavy green, "twig-like" odor, also bark- or sap-like with a fruity undertone.

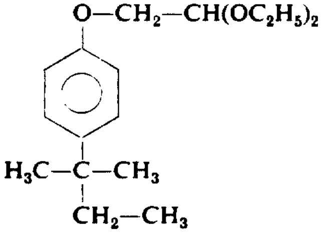
Has been suggested as a "green" modifier where the green notes should be more woody, barklike, less foliage-like.

Interesting in Lilac, Rose and even in non-floral fragrance types (Chypre, etc.).

Prod. from *para-tertiary*-Amyl phenol in weak NaOH plus Monochlordimethylacetal= $CH_2ClCH(OCH_3)_2$ to make the Acetal. Oxalic acid hydrolysis will yield the Aldehyde.

86-125;

## 207: para-tertiary-AMYL PHENOXY ACETALDEHYDE DIETHYLACETAL



$C_{17}H_{28}O_3 = 280.41$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Peculiar fruity-green, more grassy, less woody odor, as compared to the aldehyde itself. Much sweeter, not nearly as dry or harsh.

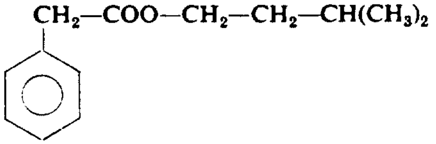
Suggested as a modifier for the Aldehyde, and in general as a "new" green odor for floral and non-floral compositions.

Prod. from *para-tertiary*-Amyl phenol in weak aqueous NaOH plus Monochloroacetal = $CH_2ClCH(OC_2H_5)_2$ to yield the Acetal.

86-125;

## 208: iso-AMYL PHENYLACETATE

*iso*-Pentyl phenylacetate.
*iso*-Amyl-*alpha*-toluate.
see NOTE below.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid. B.P. 268° C.
Sp.Gr. 0.982.

Insoluble in water, soluble in alcohol and oils.

Sweet and very tenacious, musky-animal odor with a fruity-balsamic undertone reminiscent of (fresh) Cocoa beans.

There is a considerable variation in the odor of commercial products from different suppliers of this ester.

Used in Carnation and other perfume compositions for its sweetness, fruity, almost rosy notes, delicate floralness and good performance in talcum and other functional products.

Finds extensive use in flavor compositions for imitation Butter, Chocolate, Cocoa, Honey, Licorice, Peach, etc.

With traces of Castoreum it introduces interesting effects in Cocoa, and with Anethole it gives naturalness to Licorice flavoring. Due to its high boiling point, it performs excellently in baked goods.

Concentration in functional products (food) is up to 15 ppm.

G.R.A.S. F.E.M.A. No.2081.

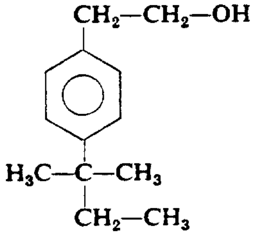
Prod. from *iso*-Amyl alcohol and Phenylacetic acid by direct esterification under azeotropic conditions.

NOTE: The ester produced from *pure n*-Pentyl alcohol has little or no trace of Cocoa-type odor, it is sweet, Honey-Apple-Rose-like.

4-10; 5-271; 44-245; 61-73; 77-194; 86-12; 103-122; 106-53; 155-88; 140-151;

## 209: para-tertiary-AMYL PHENYLETHYL ALCOHOL

*1-(4-tertiary*-Amylphenyl)ethanol.



$C_{13}H_{20}O = 192.30$

Colorless liquid. B.P. approximately 240° C.

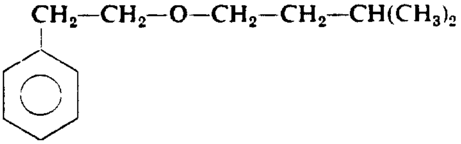
Peculiar earthy-floral, somewhat camphoraceous and rather dry odor, remotely reminiscent of Rose and Hyacinth.

Has been suggested for use in perfumery where it could introduce power (stability in soap), and modifying notes to woody-floral fragrances of the more modern soap fragrance type.

4-133;

## 210: iso-AMYL PHENYLETHYL ETHER

"Amyl phenylethyl ether" (often called)
Rhodinax.
Phenylethyl-*iso*-amylether.



$C_{13}H_{20}O = 192.30$

Colorless liquid.

Powerful Rose-Hyacinth-like odor, somewhat earthy-green, not really pleasant in the pure state, but quite attractive and interesting when diluted.

Suggested for use in floral fragrance types: Rose, Lilac, Gardenia, Hyacinth, Lily, Narcisse, etc.

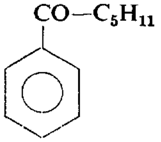
Stable in soap and other mild alkali, very stable on storage under normal conditions.

Prod. from *iso*-Amyl alcohol and Phenylethyl alcohol by dehydration.

4-10; 4-124;

## 211: AMYL PHENYL KETONE

Caprophenone.
(Commercial product is *n*-Caprophenone).



$C_{12}H_{16}O = 176.26$

Colorless liquid or crystalline mass, melting at 24-25° C. B.P. 265° C. Sp.Gr. 0.958.

*iso*-Caprophenone is a liquid at room temp.

Sweet and somewhat floral odor of great tenacity. Faintly reminiscent of Amyl salicylate, but more haylike-herbaceous.

Has been suggested for use in perfume compositions as a modifier-fixative for lower homologues (Acetophenone and derivatives, etc.) and as a modifier for the Coumarin-Amylsalicylate combination in Fougere type fragrances.

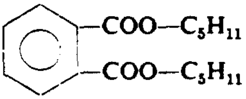
Not a very common chemical.

Prod.: from Benzonitrile plus Amyl Magnesium chloride by Grignard type synthesis.

26-410; 68-532; 86-12; 86-28; B-VII-334;

## 212: AMYL PHTHALATE

Di-*n*-amylphthalate.



$C_{18}H_{26}O_4 = 306.41$

Colorless oily liquid. Sp.Gr. 1.02.
B.P. approximately 350° C.

Insoluble in water, soluble in alcohol and oils.

Has occasionally been used as a solvent for crystalline perfume materials (Nitromusks, etv.) but does not seem to offer any significant advantage over the less expensive Diethyl phthalate, except that the former has a higher boiling point (lower vapor pressure).

Prod. from *n*-Amyl alcohol and Phthalic acid (or Phthalic anhydride).

26-478; 86-12(*iso*-Amylester);

## 213: iso-AMYL PROPIONATE

$(CH_3)_2CH—CH_2—CH_2—OOC—C_2H_5$

$C_8H_{16}O_2 = 144.22$

Colorless mobile oil. Sp.Gr. 0.87.
B.P. 161° C.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet-fruity, Apricot-Pineapple type odor with a somewhat harsh overtone and considerable radiance.

Sweet-fruity taste, reminiscent of Apricot-Banana-Pineapple.

Extensively used in flavor compositions for imitation Apple, Banana, Cherry, Grape, Peach, Pineapple, Raspberry, Rum, Strawberry, Tutti-frutti, etc.

Concentration up to 40 ppm in finished consumer product, and as high as 800 ppm in chewing gum.

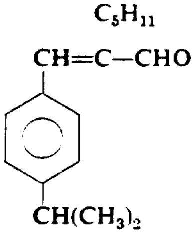
Produced from *iso*-Amyl alcohol and Propionic acid by direct esterification under azeotropic conditions.

HAZARD: This ester presents a certain FIRE HAZARD in that its flash point is about 40° C. and its vapors may form explosive mixtures with air.

G.R.A.S. F.E.M.A. No.2082.

5-231; 43-620; 90-204; 95-180; 103-106; 106-54; 128-35; B-II-141; 140-137;

## 214: alpha-**AMYL**-para-iso-**PROPYL CINNAMIC ALDEHYDE**



$C_{17}H_{24}O = 244.38$

Yellowish oily liquid. Insoluble in water, soluble in alcohol, miscible with perfume oils, poorly soluble in Propylene glycol.

B.P. 291° C. Sp.Gr. 0.95.

Herbaceous and green-spicy, fairly tenacious odor, reminiscent of vegetables and condiments.

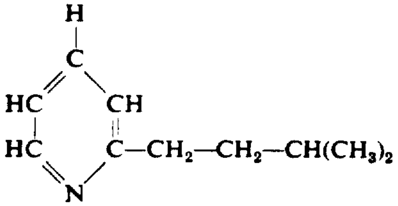
Developed in a research program aimed at new, interesting relatives to Cyclamen aldehyde, this aldehyde has at one time been available, but does not seem to be offered commercially any longer.

Its almost complete lack of floral notes limits its field of application considerably, and its overall odor type is not very interesting or attractive.

Prod.: from Heptaldehyde and Cumin aldehyde by condensation.

93-151;

## 215: alpha-iso-**AMYL PYRIDINE**



$C_{10}H_{15}N = 149.24$

Pale yellowish or almost colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

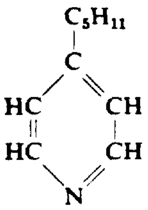
Sweet-herbaceous, slightly floral tobacco-like note, somewhat reminiscent of Elderflowers (animal undertones).

Has been suggested for use in floral fragrance compositions, but it seems that perfumers in general are hesitant to use this chemical and its homologues, probably on account of a possible skin-irritation hazard. However, the author knows of no publication specifying the hazardous effect of this chemical.

30-266; 86-72; 3-207; 159-432;

## 216: gamma-AMYL PYRIDINE

*4*-Amylpyridine.



$C_{10}H_{15}N = 149.24$

Colorless or pale yellowish liquid.

Sweet and somewhat floral odor, not without a note of animal, amine-like character. Overall less pleasant than many Alkyl pyridines, but could find use in Lilac, Honeysuckle, Narcisse and other heavy florals.

Prod. by Grignard reaction on Pyridine with Amyl bromide. Various amounts of *2*-Amyl pyridine may be formed, and the reaction must be controlled to increase the yield of the *gamma*-isomer.

86-4; See also 30-266 and 30-268;

## 217: iso-AMYL PYRUVATE

*iso*-Pentyl pyruvate.
*iso*-Amyl pyroracemate.
Pyruvic acid, *iso*-Amylester.

$(CH_3)_2CH—CH_2—CH_2—OOC—CO—CH_3$

$C_8H_{14}O_3 = 158.20$

Colorless liquid. B.P. 185° C. Sp.Gr. 0.987

Fresh ethereal caramel-Rum-like odor with fruity-floral undertones.

Sweet ethereal-fruity, caramellic taste.

Occasionally used in perfumery to introduce an ethereal topnote e.g. in citrusy Colognes, etc.

Used in flavor compositions for Arak, Fruit (Tutti-frutti), Maple, Rum, etc.

Concentration up to 12 ppm in finished product.

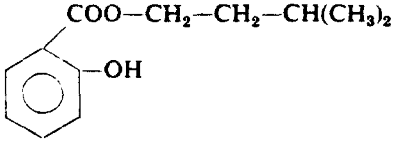
Prod. from Pyruvic acid and *iso*-Amyl alcohol by direct esterification under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2083.

3-8; 4-8; 4-10; 77-192; 86-12;

## 218: iso-AMYL SALICYLATE

*iso*-Pentyl salicylate.
*iso*-Pentyl-*ortho*-hydroxybenzoate.
"Tresseine" (A. Boake, Roberts & Co., Ltd.).
Trefle.
Orchidee.
Trefol.
Amyl salicylate (most commonly called).



$C_{12}H_{16}O_3 = 208.26$

Colorless oily liquid. Sp.Gr. 1.06.
B.P. 277° C.

Insoluble in water, soluble in alcohol, perfume and flavor materials.

Sweet herbaceous-green, slightly floral odor. Very tenacious, somewhat woody-earthy, sweet dryout notes. Refined qualities of this ester may show a marked difference in odor, particularly richer in sweetness and floral tones.

Peculiar herbaceous-"perfumey" flavor.

Extensively used in floral and non-floral perfume types: Very often in Carnation, Hyacinth, Orchid, Trefle, and almost inevitably in Fougere types. Its low cost and worldwide availability makes it one of the most important perfume chemicals.

Occasionally used in "Root Beer" type flavors and certain Fruit flavors. Concentration is usually mere traces (a few ppm in finished consumer product).

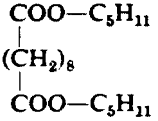
Prod. from *iso*-Amyl alcohol and Salicylic acid by direct esterification with a catalyst and usually under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2084.

4-10; 5-236; 44-788; 44-789; 77-193; 95-188; 96-207; 85-27; 103-122; 103-155; 106-55; 156-325;

## 219: iso-AMYL SEBACATE

*iso*-Pentyl decanedioate.
*iso*-Amyl-*1,8*-octanedicarboxylate.
Di-*iso*-amylsebacate.



$$\begin{array}{l} COO-C_5H_{11} \\ | \\ (CH_2)_8 \\ | \\ COO-C_5H_{11} \end{array}$$

$C_{20}H_{38}O_4 = 342.52$

Colorless leafy crystals. Insoluble in water, soluble in alcohol, miscible with oils.

Very faint waxy-fatty odor, or practically odorless.

Has been suggested as a modifier-fixative in certain flower bases, as a blender in Orris-type fragrances, as an extender for Ionones, etc. Does not seem to contribute significantly to the overall odor of such compositions.

Prod. from Sebacic acid (from Castor oil by alkali heating and distillation) with *iso*-Amyl alcohol, direct esterification.

4-10; 3-9;

## 220: AMYL STEARATE

Amyl octadecanoate.
see NOTE below.

$C_{17}H_{35}COO-C_5H_{11}$

$C_{23}H_{46}O_2 = 354.64$

Colorless oily liquid. Solidifies in the cold and melts at 14° C. Sp.Gr. 0.855.

Insoluble in water, soluble in alcohol and oils.

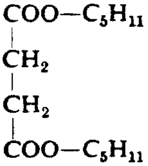
Virtually odorless, useful as a solvent, but does not seem to offer significant advantages over the much less expensive Diethyl phthalate.

NOTE: The *iso*-Amyl stearate has M.P. 23° C. and is poorly soluble in alcohol.

3-9; 4-10; 26-410; B-II-380;

## 221: iso-AMYL SUCCINATE

Di-*iso*-amyl succinate.



$$\begin{array}{l} COO-C_5H_{11} \\ | \\ CH_2 \\ | \\ CH_2 \\ | \\ COO-C_5H_{11} \end{array}$$

$C_{14}H_{26}O_4 = 258.36$

Colorless oily liquid. B.P. 290° C.
Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

Pleasant, mild, aromatic odor, suggestive of Gooseberry with a Grape-like, winey undertone, but overall weak.

Very mild fruity taste, reminiscent of juices of tart berries.

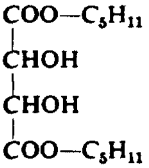
Has been suggested for use in imitation fruit flavors, but this ester is not specifically mentioned as permitted for food flavors in the U.S.A. It is commonly used elsewhere for imitation Blackcurrant, Gooseberry, Brandy, Arrak and other flavor types.

Prod. from *iso*-Amyl alcohol and succinic acid by direct esterification under azeotropic conditions.

4-10; 26-478; 86-12; B-II-611; 140-146;

## 222: AMYL TARTRATE

Di-*iso*-Amyl tartrate.



$$\begin{array}{l} COO-C_5H_{11} \\ | \\ CHOH \\ | \\ CHOH \\ | \\ COO-C_5H_{11} \end{array}$$

$C_{14}H_{26}O_6 = 290.36$

Colorless liquid. Sp.Gr. 1.06.
B.P. approximately 300° C.

Insoluble in water, soluble in alcohol and oils.

Very faint odor, remotely reminiscent of Brandy, nondescript fruity.

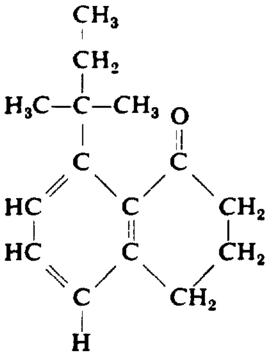
Has been suggested as a fixative for Brandy and Cognac flavors, but does not seem to contribute much to such compositions.

Prod. by direct esterification of *iso*-Amyl alcohol with Tartaric acid under azeotropic conditions.

4-10; 26-478; B-III suppl.-179;

## 223: 8-tertiary-AMYL-1-TETRALONE

*8-tertiary*-Amyl-*alpha*-tetrahydronaphthalone.



$C_{15}H_{20}O = 216.33$

Colorless viscous liquid. Insoluble in water, soluble in alcohol and oils.

Dry-woody, somewhat camphoraceous odor.

Suggested for use in artificial Patchouli oil, Sandalwood compositions, etc.

This chemical is rarely offered under its proper chemical name.

see also: 30-252; 68-1344;

## 224: AMYL THIOGLYCOLATE

Amyl mercapto acetate.

$HS-CH_2-COO-C_5H_{11}$

$C_7H_{14}O_2S = 130.19$

Colorless oily liquid. Sp.Gr. 1.006.

When absolutely free from Thioglycollic acid, this ester has a faint, but pleasant aromatic-herbaceous odor, remotely reminiscent of Amyl acetate.

However, it does not offer any unique fragrance notes that would justify its wider application in fragrances or flavors.

It should be kept in mind that Thioglycollic acid liberates Hydrogen sulfide under acid conditions. This presents a certain hazard in the use of all esters of Thioglycollic acid.

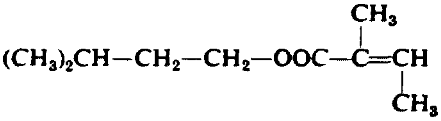
When the acid was introduced in cosmetic preparations (cold wave etc.) more than 20 years ago, many esters were prepared in the research for new fragrance types. The Amyl ester is one of these.

Produced from (*iso*-)Amyl alcohol and Thioglycollic acid by direct esterification under azeotropic conditions (no catalytic acid added).

34-1245;

## 225: iso-AMYL TIGLATE

*iso*-Pentyl-*trans-alpha*-Methyl crotonate.
*iso*-Amyl-*trans-alpha-beta*-Dimethylacrylate.
see Note below.



$$(CH_3)_2CH-CH_2-CH_2-OOC-\overset{CH_3}{C}=\underset{CH_3}{CH}$$

$C_{10}H_{18}O_2 = 170.24$

Colorless liquid. B.P. 200° C.

Herbaceous-winey, overall pleasant odor reminiscent of sweet medicinal herbs (meadowlike odor). The odor bears quite some resemblance to that of the -angelate.

The taste is similar to the odor at dilutions below 10 ppm.

Since Tiglic acid is the more stable isomer (more than Angelic acid) there is reason to believe that the Tiglates will become increasingly popular in the formulation of artificial essential oils. Recent years' investigations have confirmed the presence of these esters in a great number of very important, and many expensive, essential oils.

The ester could also find use in flavor compositions, particularly for Liqueur flavors.

Prod. from *iso*-Amyl alcohol and Tiglic acid by direct esterification under azeotropic conditions.

Note: Commercial Angelic (Tiglic) acid has usually contained a large amount of the other isomer. Esters prepared from such acid would accordingly consists of a mixture of the two isomers. However, recent methods of synthesizing the two acids have brought comparatively pure and lower cost acids on the market.

66-636; 90-223;

## 226: iso-AMYL UNDECYLATE

*iso*-Pentyl undecanoate.

$(CH_3)_2CH—CH_2—CH_2—OOC(CH_2)_9CH_3$

$C_{16}H_{32}O_2 = 256.43$

Colorless oily liquid. Insoluble in water, miscible with alcohol and oils.

Oily-rosy odor with vinous-brandylike undertone, overall mild and by some observers described as "odorless".

However, this ester does contribute perceptible and interesting flavor and fragrance notes to compositions containing lower boiling (more volatile) ingredients.

The ester finds some use in perfumery where it can introduce quite natural and round, pleasant "mellow" notes in herbaceous or citrus type fragrances, or in Rose, Sweet Pea and other florals as a modifier in the "waxy" petal complex.

Used more frequently in flavor compositions for imitation Rum, or for Butterscotch, Chocolate, Brandy, etc.

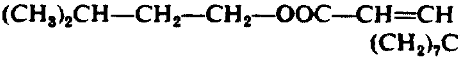
Concentration is usually limited to traces due to the great power of this ester in flavors.

Prod. by direct esterification of *iso*-Amyl alcohol with Undecanoic acid under azeotropic conditions. To wash the ester free from the acid with weak alkali, it may be necessary to extract the ester from the mixture (emulsion is almost inevitably formed) with a non-polar, volatile solvent and recover the ester free from solvent.

4-10; 38-I-604; 103-122;

## 227: iso-AMYL UNDECYLENATE

*iso*-Pentyl undecenoate.



$$(CH_3)_2CH—CH_2—CH_2—OOC—CH=\underset{(CH_2)_7CH_3}{CH}$$

$C_{16}H_{30}O_2 = 254.42$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Somewhat fatty-green, oily and fruity, Apricotlike odor with a faintly floral (Rose) undertone. Pronounced brandylike, winey-herbaceous in high dilution, but becomes rather unpleasant, almost "rubberlike" at high concentrations.

Probably not used very frequently in perfumes.

Finds extensive use in flavor compositions, where its high boiling point makes it an excellent fixative for Rum and Brandy flavors for hard candy, baked goods and other functional products the preparation of which involves heat. Many "oil soluble" Rum flavors contain this ester and owe their power to it.

Prod. by direct esterification of *iso*-Amyl alcohol with Undecy*lenic* acid (a product from Castor oil distillation) under azeotropic conditions. The ester is extracted from the alkali washings with a volatile, non-polar, harmless solvent.

3-9; 3-37; 3-61; 4-10; 38-I-604; 103-121;

## 228: AMYL VALERATE

*n*-Amyl-*n*-valerate.
*n*-Pentyl-*n*-pentanoate.
NOTE: The most common commercial ester is the *iso*-Amyl-*iso*-Valerate.

$CH_3(CH_2)_3CH_2—OOC(CH_2)_3CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. B.P. 188° C.

Fruity-ethereal, heavy, Apple-like odor, not as fresh-druity as the *iso*-Amyl-*iso*-valerate.

Sweet Apple-like taste, somewhat harsher than that of the *iso*-Amyl-*iso*-valerate.

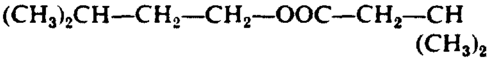
Finds some use in flavor compositions, but is not as popular as the isomer which is furthermore less expensive.

Prod. from *n*-Amyl alcohol and *n*-Valeric acid by direct esterification under azeotropic conditions.

96-215;

## 229: iso-AMYL-iso-VALERATE

*iso*-Pentyl-*iso*-valerate.
*iso*-Amyl valerianate.



$$(CH_3)_2CH—CH_2—CH_2—OOC—CH_2—\underset{(CH_3)_2}{CH}$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. B.P. 190° C. Sp.Gr. 0.858.

Very slightly soluble in water, miscible with alcohol and oils.

Peculiar fruity odor reminiscent of ripe apples, or more like the overwhelmingly choking odor of apples stored in a warehouse, almost a "fermented" apple odor.

Fresh-fruity taste, reminiscent of apple rind. Also of raspberry.

Finds extensive use in flavor compositions, primarily in imitation Apple, and in the related "wine" or "Champagne" type imitation flavors for soft candy, beverages, etc. Further as a modifier in imitation Apricot, Banana, Cherry, Honey, Peach, Pineapple, Mango, Raspberry, Strawberry, Walnut – and in combination flavors such as Cream Soda, Tutti-frutti, Rum and in Vanilla.

A specific use is the application in imitation Gooseberry flavor. Concentrations are usually around 50-60 ppm, except in chewing gum, where it may be as high as 400 ppm. (Calculated on functional consumer product).

Prod.

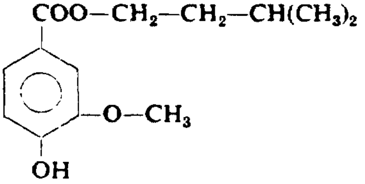
1) by direct esterification of *iso*-Amyl alcohol with *iso*-Valeric acid under azeotropic conditions.
2) by controlled oxidation of *iso*-Amyl alcohol with Potassium dichromate-Sulfuric acid mixture.

G.R.A.S. F.E.M.A. No.2085.

4-11; 26-412; 33-932; 33-933; 90-211; 95-181; 77-20; 77-186; 103-123; 128-37; B-II-312; 140-141;

## 230: iso-AMYL VANILLATE

*iso*-Amyl-*4*-hydroxy-*3*-methoxybenzoate.



$C_{13}H_{18}O_3 = 222.29$

Colorless oily liquid. Almost insoluble in water, slightly soluble in alcohol, soluble in most oils.

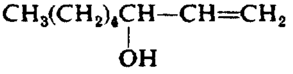
Very faint balsamic-animal odor with floral undertones.

The title ester finds limited use in perfume compositions, occasionally in Oriental bases with Civet and Tolubalsam, or in novel creations where its fixative effect and peculiar, but rather faint odor can be utilized.

Prod.: from Vanillic acid and *iso*-Amyl-alcohol.

## 231: AMYL VINYL CARBINOL

*1*-Octen-*3*-ol.
*3*-Octenol.
Matsutake alcohol.
*n*-Pentyl vinylcarbinol.
(*laevo-, dextro- and dl*-forms are all known).



$CH_3(CH_2)_4\underset{OH}{CH}-CH=CH_2$

$C_8H_{16}O = 128.22$

Colorless liquid. B.P. 175° C. Sp.Gr. 0.84.

Very powerful, sweet-earthy, almost buttery and fungus- or fermentation-like odor with a strong herbaceous note, suggestive of Lavender-Lavandin-Rose and Hay. Somewhat acrid-chemical undertone which is hardly perceptible at proper (high) dilution.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, haylike-earthy taste.

Since this chemical has been identified in Lavandin and many other important essential oils, it has become extremely popular in the art and science of preparing artificial or "reconstituted" essential oils. This is where the alcohol finds its main outlet.

Also used in flavors (and in artificial Spearmint), such as Spice, Fruit, etc. usually in very low concentration: 0.2 to 6 ppm in the finished consumer product.

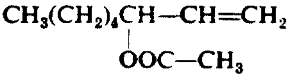
Prod. by Vinyl Grignard reaction on Hexaldehyde – or from Amyl Magnesium Bromide plus Acrolein.

G.R.A.S. F.E.M.A. No.2805.

4-10; 10-35; 12-62; 45-402; 87-485; 156-16; 146-17;

## 232: AMYL VINYL CARBINYL ACETATE

*3*-Acetoxy octene.
*beta*-Octenyl acetate.
Octenyl acetate (Comp. Parento).
*1*-Octen-*3*-yl acetate.
*n*-Pentyl vinyl carbinyl acetate.
"Amyl crotonyl acetate".



$CH_3(CH_2)_4\underset{OOC-CH_3}{CH}-CH=CH_2$

$C_{10}H_{18}O_2 = 170.26$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.89. B.P. 190 C.

Fresh-herbaceous, fruity-minty odor, recalling the topnotes in Lavender and Lavandin (and many other herbaceous essential oils) less warm and not buttery as the alcohol, more citrusy, and almost geranium-like in topnote. Some observers find a rosy note in this ester.

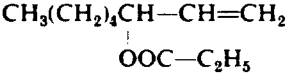
Extensively used in the "reconstitution" of essential oils, in which it may enter at concentrations up to 1 or 2 percent. It is free from the mushroom-like odor of the alcohol and therefore somewhat more versatile in use.

Prod. by Acetylation of Amyl vinyl carbinol (preferably the *dextro*-Octenol).

2-717; 4-10; 90-222; 156-16; 156-17;

## 233: AMYL VINYL CARBINYL PROPIONATE

*n*-Pentyl vinyl carbinyl propionate.
*3*-Propoxy octene.
*beta*-Octenyl propionate.
*1*-Octen-*3*-yl propionate.



$$\underset{\displaystyle \quad\quad OOC{-}C_2H_5}{CH_3(CH_2)_4CH{-}CH{=}CH_2}$$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Fruity-herbaceous, almost haylike-sweet odor, recalling topnotes in Lavender-Clary Sage. Less Lavandin-like, more Lavender-Clary-Sage-like than the Acetate, and also sweeter-warmer.

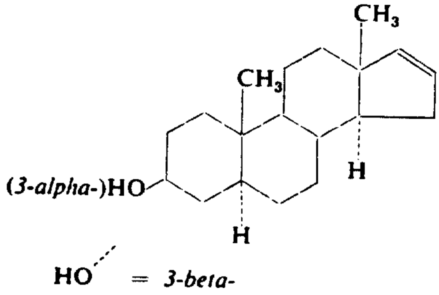
This ester, which is barely available (1967) could have an interesting future as a "new" note in perfumes, particularly for the growing market of Men's fragrances. Even at the level of a few percent in herbaceous-citrusy fragrance bases, it makes itself perceptible and presents generally desirable notes.

Could also find use in the "reconstitution" of certain essential oils.

Prod. from Amyl vinyl carbinol by esterification with Propionic acid or Propionic anhydride.

Information: Takasago Perfumery Company, 1967. No literature.

## 234: 3-alpha-**ANDROSTENOL** and 3-beta-**ANDROSTENOL**



$C_{19}H_{30}O = 274.45$

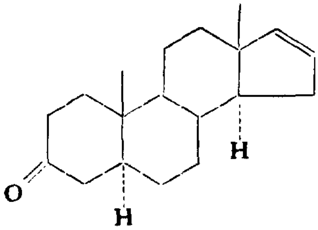
*3-alpha-* has a strong musky odor.
*3-beta-* has only a weak musky odor.

See comments under monograph: Androstenone.

4-12; 30-279; 30-280; 86-13; 159-450;

## 235: Δ16-ANDROSTENONE-3

A chemical related to Civettone.



$C_{19}H_{28}O = 272.45$

Reported as having a penetrating urine-like odor.

A fairly large number of sex hormones, some of which are listed in this handbook (see Allopregnanol, Allopregnenone, etc.) have been suggested for use in fragrances for quite obvious purposes.

It is beyond doubt, however, that these chemicals have great academic interest in the study of olfaction, the relation between olfaction and chemical structure, and the influence of odors upon human Nature and behaviour.

Results from these studies are unfortunately often published in the highly scientific type of chemical papers or booklets, mostly issued by Universities, and very rarely reaching the creative perfumer's desk or laboratory.

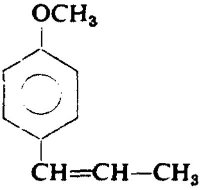
The following periodicals have frequently brought such reports:

Journal of biological Chemistry.
Helvetica Chimica Acta.
Chemistry and Industry.
Journal of American Chemical Society.
Journal of organic Chemistry.
Chemische Berichte.
Nature.
Biochemical Journal.

See also: 4-12; 30-279; 67-919; 159-450;

## 236: ANETHOLE

*trans*-Anethole.
*iso*-Estragole.
*para*-Propenyl phenyl methylether.
*para*-Propenyl anisole.
*1*-Methoxy-*4*-propenyl benzene.
*para*-Methoxy-*alpha*-phenyl propene.
"Anise camphor" (old name).
(exists in *cis*- and *trans*-form).



$C_{10}H_{12}O = 148.21$

Colorless, slightly oily liquid. Sp.Gr. 0.99. B.P. 236° C.

Slightly soluble in water, miscible with alcohol and oils, poorly soluble in Propylene glycol and Glycerin.

Solidifies in the cold, melts at 23° C (21-22° C.).

A melting point of +20° C corresponds to 3.6% *cis*-isomer in the Anethole.

Very sweet, herbaceous-warm odor, sweet taste. It is the prototype of odors described as "anisic".

Extensively used in low-cost fragrances as a sweetener, particularly in soap perfumes and household product fragrances, industrial fragrances, etc. Blends very well with many florals of the Lilac, Appleblossom-type, and with non-florals such as Fougeres and woody types.

Very extensively used in flavor compositions (NOTE: *trans*-Anethole only) where its enormously flexible concentration level makes it an almost ideal flavor base. This is pictured in chewing gum and the heavily flavored French alcoholic beverage known as "Anisette", where concentrations may run as high as 1500 ppm.

The FDA "White List" permits the use of *Anise oil* in concentrations up to 3500 ppm. (Anise oil contains more than 90% Anethole). Anethole forms the standard flavoring ingredient in Licorice candy, so common that

Anise odor is often classified as "Licorice odor" by the layman. Anethole is furthermore used in Birchbeer flavor, Fruit, Honey, Liquor, Nut, Rootbeer, "Sarsaparilla", Spice, Vanilla, etc.

Anethole is stable under normal storage conditions, but may oxidize under poorer conditions and form *4:4*-Dimethoxystilbene or it may polymerize to Metanethole, etc.

G.R.A.S. (*trans*-Anethole only; *cis*-Anethole is considered 15 times more toxic and possibly hazardous to human beings at normal use concentrations).

F.E.M.A. No.2086.

Prod.:

1) by Isomerization of Estragole using alcoholic Potassium hydroxide as agent.
2) From Anisole (Methyl phenylether) plus Propionaldehyde, Hydrochloric acid and Phosphoric acid to yield *alpha*-Chloro-*para*-propylanisole which is reacted with Pyridine to produce Anethole.
3) From Anisaldehyde and Ethylmagnesium iodide.
4) By isolation directly from Star Anise seed oil or Anise oil.

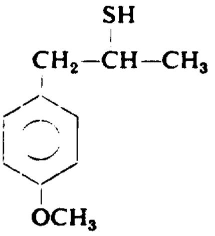
Methods 1) and 2) are the most important in the U.S.A., while method 4) can be practised in areas of availability of Star Anise oil at low cost.

Total Anethole content: 94% or higher. Anethole from Estragole contains considerable amounts of *cis*-Anethole which must be removed (e.g. by careful fractionation) before the Anethole is suitable for food use. The *cis*-isomer appears in the foreruns of the distillation. The odor of *cis*-Anethole is more Fennel-like, camphoraceous and generally unpleasant as compared to that of *trans*-Anethole.

4-12; 27-49; 65-509; 65-510; 67-397; 68-969; 85-27; 86-13; 90-420; 77-199; 100-79; 106-56; B-VI-566; 140-170;
Arizona Chemical Comp. data sheet, Aug. 1966.

## 237: ANETHOLE MERCAPTAN

Presumably: *1*-(*para*-Methoxy phenyl) propane-*2*-thiol. with related chemicals as minor impurities.



$C_{10}H_{14}OS = 182.22$

Almost colorless slightly oily liquid.
Sp.Gr. 1.05.

Pleasant, sweet-herbaceous odor, perhaps less sweet than Anethole, but with a freshness instead.

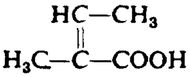
This chemical is being suggested for use in fragrances and flavors.

For these purposes, however, the material is still under experimental use by the consuming industries, and it is too early to make any firm statements as to the future aspects of Anethole mercaptan. (1968).

(Phillips Petroleum Comp., Bartlesville, Oklahoma 74003, U.S.A. – data sheet 1.G.66 – Oct. 1966).

## 238: ANGELIC ACID

*cis-alpha*-Methyl crotonic acid.
*cis-2*-Methyl-*2*-butenoic acid.
*cis-2*-Methyl crotonic acid.
*cis-2,3*-Dimethyl acrylic acid.
This is the less stable form of the Pentenoic acid:
(See also: Tiglic acid, the more stable form).



$$\begin{array}{l}\quad\ HC-CH_3\\ \quad\ \ \ \|\\ H_3C-C-COOH\end{array}$$

$C_5H_8O_2 = 100.11$

White crystals, melting at 46° C. B.P. 185° C. Sp.Gr. 0.95 (liq.).

Volatile with steam, slightly soluble in water, soluble in alcohol and oils. The aqueous solution will eventually isomerize to Tiglic acid upon standing.

Peculiar spicy-caramellic, slightly acid odor. Herbaceous-acid taste, pleasant at proper dilution.

The acid itself does not find much use in perfumery beyond that of being a trace ingredient in artificial or "reconstituted" essential oils, where it may have been identified by analysis of the natural oil.

Its esters find more extensive use in perfumes and flavors. (Ethyl angelate, Butyl angelate, Amyl angelate, etc.).

The acid is occasionally used in flavor compositions, but due to the poor stability of the aqueous solution, the Tiglic acid is preferred over the Angelic for flavor work.

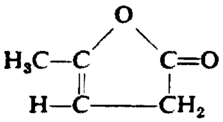
Prod.: Among many methods known, one uses *2*-Hydroxy-*2*-butyronitrile to produce Tiglic acid, from which Angelic can be made by Bromine treatment. Another method goes directly from *alpha*-Hydroxy-*alpha*-methylbutyric acid which by dehydration yields Angelic acid, or a mixture of Angelic and Tiglic acids.

26-512; 66-635; 100-80; B-II-428; 140-144;

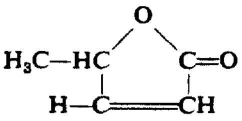
## 239: ANGELICA LACTONE

The *alpha*-Angelicalactone is sometimes called *beta-gamma*-Angelicalactone, and the *beta*-Angelicalactone is sometimes called: *alpha-beta*-Angelicalactone.

NOTE: Do not confuse this chemical with Cyclopentadecalactone, which occurs naturally in Angelica root oil and sometimes is called "Angelica lactone". See Cyclopentadecanolide.



*alpha-*



*beta-*

$C_6H_6O_2 = 98.10$

*alpha-:*
*gamma*-Methyl-*beta-gamma*-crotonolactone
or: *5*-Methyl-*2,3H*-furanone.
Needle-like crystals, M.P. 18° C.
B.P. 170° C.
Soluble 5 % in water.
Modestly toxic, 10 grams may kill an adult man.

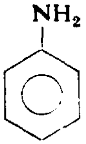
*beta-:*
*gamma*-Methyl-*alpha-beta*-crotonolactone
or: *5*-Methyl-*2,5H*-furanone.
Liquid, Sp.Gr. 1.08. B.P. 200° C.
Soluble in water.
Non-toxic.
Prod. by dry distillation of Levulinic acid.

This lactone finds occasional use in the reconstitution of essential oils. Its intensely sweet-herbaceous, almost tobacco-like odor makes this chemical interesting for application in new fragrance types. However, it would be wise to investigate its pharmacological and dermatological properties first.

85-28; 100-80; 66-845;

## 240: ANILINE

Phenyl amine.
Aminobenzene.
Aminophen.



$C_6H_7N = 93.13$

Colorless oily liquid, solidifying in the cold. M.P. −6° C. Sp.Gr. 1.02. B.P. 184° C.

3.5% soluble in cold water, slightly better in hot water. Miscible with alcohol and oils.

When absolutely pure, this material has a warm, sweet and actually pleasant odor – in suitable dilution. Commercial grades are often unsuitable for smelling because of traces of very ill-smelling Amines and other off-odors, by-product, etc.

This Amine has been suggested for use in Oriental fragrances, but the author hopes that it stays with the suggestion only. There is no reason to use Aniline in perfume compositions, but there are many reasons not to use it:

The title material is considered moderately toxic. 0.25 grams is a serious dose for adult human beings.

It is chemically reactive and may cause considerable disturbances in a perfume composition. It forms adducts with aldehydes, ketones, acids, etc.

Aniline discolors easily under exposure to daylight. Although the discoloration is usually ascribed to the presence of trace impurities in the Aniline, it is safe to assume that commercial material is so impure that it presents a discoloration hazard.

Aniline is flammable, although not presenting an explosion hazard.

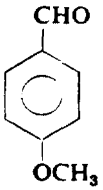
Briefly, it should be banned from the perfumer's shelf, just as well as Nitrobenzene.

Prod.: from Benzene via Nitrobenzene, followed by reduction with Iron in Hydrochloric acid to Aniline.

26-412; 68-163; 100-82; 160-798; 163-63; B-XII-59;

## 241: ANIS ALDEHYDE

*para*-Anisaldehyde.
*para*-Methoxy benzaldehyde.
*para*-Hydroxybenzaldehyde methylether.
"Aubepine".
"Aubepine liquid".
Anisal.
Anisic aldehyde.



$C_8H_8O_2 = 136.15$

Colorless or pale yellowish liquid. Solidifies in the cold, melts at 2°,5 C.

Soluble 0.3% in water, miscible with alcohol and oils, poorly soluble in Propylene glycol and Glycerin.

B.P. 248° C. Sp.Gr. 1.12.

Intensely sweet floral, yet somewhat "hay-like" odor, generally described as Hawthorne-like.

Sweet herbaceous-spicy taste.

Very widely used in perfumery, only restricted because of its poor stability in alkali and in the presence of Amines. Certain fragrance types may contain well over 10% of this aldehyde, while a few percent or less can introduce satisfactory effects in other types. It is an excellent companion to the sharper aldehydes, will round them off and reduce their pungency.

Occasionally used in flavor compositions where its sweetness makes it quite versatile:

Anise, Apricot, Butter, Caramel, Cherry, Chocolate, Black Walnut, Nut, Peach, Raspberry, Strawberry, Spice, Vanilla, Walnut, – and often as a modifier in Peppermint flavor combinations for chewing gum.

Concentrations usually 0.5 to 30 ppm in finished goods, and up to 75 ppm in chewing gum. The flavor threshold for Anisaldehyde on the average panel person is about 0.2 ppm. (Single chemical in Sugar water).

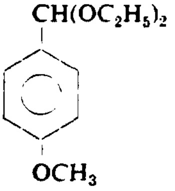
The aldehyde may oxidize in air to *para*Anisic acid and lose its odor.

Prod. from Anethole, or from Estragole(*iso*-Anethole), or from Cresol, or from *para*-Hydroxybenzaldehyde.

G.R.A.S. F.E.M.A. No.2670.

4-12; 5-115; 26-414; 27-53; 29-46; 31-61; 34-679; 65-358; 68-744; 85-28; 100-83; 103-266; 106-57; B-VII-67; 156-33; 140-162;

## 242: ANISALDEHYDE-DIETHYLACETAL



$C_{12}H_{18}O_3 = 210.28$

Colorless liquid. B.P. 263° C. Sp.Gr. 0.99.

Mild floral-sweet odor, slightly green, herbal note.

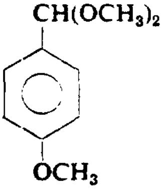
Suggested for use in Lilac fragrances, Alpine Violet, Heliotrope, Honeysuckle, Appleblossom, Sweet Pea, etc.

This Acetal has an odor distinctly different from that of the parent aldehyde, and the Acetal is much weaker of odor. It is most conceivable that the Acetal can not fill in any important place on the perfumer's shelf.

Produced from Anisaldehyde and Ethyl alcohol.

86-13;

## 243: ANISALDEHYDE-DIMETHYLACETAL



$C_{10}H_{14}O_3 = 182.22$

Colorless liquid. B.P. 235° C. Sp.Gr. 1.08.

Herbal-green, somewhat floral odor, suggestive of Lilac ("Lilac-green"), Hyacinth, Appleblossom, etc.

Drier than the Diethyl acetal.

Probably of very limited interest to the perfumer. The odor is weaker than that of the parent aldehyde, and quite different of type.

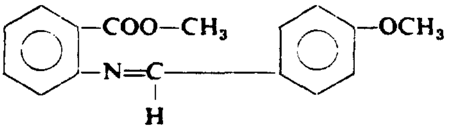
Prod. from Anisaldehyde and Methyl alcohol.

86-13;

## 244: ANISALDEHYDE-METHYLANTHRANILATE

"Acaciol".

A "Schiff's base".



$C_{16}H_{15}NO_3 = 269.30$

Very viscous, intensely yellow liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol or Glycerin.

Heavy-sweet, intensely floral odor with fruity undertones. Resembling the odor of the flowers of Robinia pseudoacacia, remotely resembling notes in Gardenia (fruity-Peach-like notes).

Used in perfumes of the heavy floral type, and the "powdery"-floral type: Acacia, Mimosa, Honeysuckle, Jasmin, Gardenia, etc. Its extraordinary tenacity makes it necessary to blend this material with suitable fixatives of similar vapor pressure to prevent the Acaciol from dominating the dryout-notes of the composition.

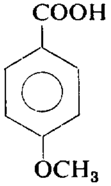
Probably not used in flavors.

Prod. by condensation of Anisaldehyde with Methyl anthranilate. Water is removed by gentle vacuum during the reaction.

7-4; 7-367; 86-1; 103-162; 155-80; see also Amer.Perf. Sept. 1948, p. 218-220.

## 245: ANISIC ACID

*para*-Anisic acid.
*para*-Methoxybenzoic acid.
"Draconic acid" (old name).
"Umbellic acid" (old name).



$C_8H_8O_3 = 152.15$

White crystals. M.P. 184° C. B.P. approximately 280° C.

Soluble 0.04% in cold water, slightly soluble in hot water. Soluble in alcohol and oils.

Practically odorless when pure, this chemical may carry some odor from the starting material (Anethole, or other).

As such, the acid has very little importance to the perfume or flavor industry. It has some interest in that it is an isomer (empirical) of a very popular fungistat, Methyl-*para*-hydroxybenzoate.

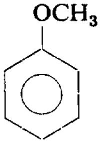
Anisic acid does influence the flavor of a composition in which it is incorporated, but it does not seem to contribute interesting notes or great power.

Prod. (many methods) e.g. by oxidation of Anethole.

26-596; 68-769; 90-500; 96-201; 100-83; B-X-154; 140-152;

## 246: ANISOLE

Methoxybenzene.
Methyl phenyl ether.
Phenyl methyl ether.
NOTE: Do not confuse this chemical with Anethole.



$C_7H_8O = 108.14$

Colorless liquid. B.P. 154° C. Sp.Gr. 0.996.

Insoluble in water, soluble in alcohol and oils.

Powerful and harsh, yet very sweet odor, rather chemical and not reminiscent of any natural material, except perhaps remotely of Anise. Its odor is often classified as "anisic", but the author finds that this term would not be used by perfumers.

This ether finds some use in low-cost fragrances, where power is important, industrial masking odors, etc. It is stable in alkali and mild acid, and therefore quite suitable for this type of fragrance application.

Suggested for use – and actually used – in a number of flavor types: Birch Beer, "Licorice", Root Beer, "Sarsaparilla" and Wintergreen, but the author has a strong suspicion that many of these uses have come up because of confusion of Anisole with Anethole, which is the natural item to use in all of the named flavor types. Anisole is – in the author's opinion – NOT a substitute for Anethole.

Prod. from Phenol in mild aqueous alkali with Dimethyl sulfate.

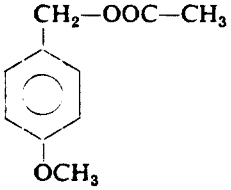
G.R.A.S. F.E.M.A. No.2097.

26-414; 68-426; 85-28; 90-375; 100-83; 103-266; 106-59; B-VI-138;

## 247: ANISYL ACETATE

*para*-Methoxy benzyl acetate.
"Cassie ketone".

NOTE: The author feels that a confusion with Anisyl acetone is apparent in the case of "Cassie ketone", this name being more obvious for Anisyl acetone than for the acetate. However, the name "Cassie ketone" is used for the acetate perhaps because the error once was made and never corrected, but repeatedly quoted in perfumery literature.



$C_{10}H_{12}O_3 = 180.21$

Colorless liquid. Insoluble in water, Propylene glycol and Glycerin. Soluble in alcohol and oils. B.P. 235° C. Sp.Gr. 1.10-1.11.

Mild fruity-floral, slightly balsamic-vanilla-like odor in the Plum and Lilac type, also reminiscent of certain types of Cherry.

Excellent in sweet florals such as Lilac, Acacia, Mimosa, Violet, Honeysuckle. It is one of the classic ingredients to achieve the so-called "powdery" notes which are still in strong demand by the fragrance consumers. In combination with Cyclamal it produces very unusual, powerful and pleasant effects of this type.

Frequently used in flavor compositions for imitation Berry, Chocolate, Cocoa, Fruit, (Cherry), Vanilla, etc.

Concentrations usually about 30 ppm. This ester performs very well in baked goods (heat-stable).

Prod. from Anisyl alcohol (the quality of this in *most important*!!) by direct esterification with Acetic acid or Acetic anhydride.

G.R.A.S. F.E.M.A. No.2098.
FCC 1964-787.

4-12; 5-63; 77-184; 103-96; 106-61; 140-137;

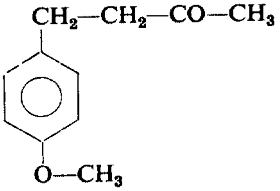
## 248: ANISYL ACETONE

*para*-Methoxy phenylbutanone (common commercial name).
*para*-Methoxy benzylacetone.
4-(*para*-Methoxyphenyl)-2-butanone.
"Frambinone methylether".
"Raspberry ketone Methylether".
"Methyl Oxanone".

NOTE: Considerable confusing prevails in literature descriptions of the chemical bearing the name Anisyl acetone.

Acknowledged chemical reference books use the title name for Methoxy phenyl *acetone*, but the author of this work would insist that Methoxy phenyl *butanone* is the correct name for it.

Methoxy phenyl acetone would be Anisyl methyl ketone, sometimes called Anisic ketone. That chemical is described in the present work under the title name of: *para*-Methoxyphenyl acetone.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid. B.P. 277° C. Solidifies in the cold, melts again at 10° C.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Intensely sweet, floral and slightly fruity, Cherry-preserve-like odor of good tenacity. It has considerable resemblance to Heliotropine in its overall performance in a composition. The main difference is in the fruity character, which is described as "Raspberry-like" by some perfumers (while Heliotropine is more "Cherry-like") and in the lack of "powdery" notes in the title material as compared to Heliotropine.

Pleasant, sweet-fruity, Cherry-Raspberry-type flavor at concentrations below 40 ppm. Tends to appear "perfumey" at levels higher than 100 ppm.

This ketone, a methylether of a very popular material (see *para*-Hydroxy phenylbutanone), finds use in perfume compositions as a modifier for Heliotropine, a sweetener for Cyclamen aldehyde, and a blender in many types of sweet florals, Fougères, Oriental fragrances, etc. It suffers from the drawback of being considerably more expensive than Heliotropine, and it can therefore not truly be classified as a substitute for that material. It shows less tendency of discoloration in combination with the materials normally causing such trouble with Heliotropine.

The material is also used in flavor compositions, particularly in Raspberry and Cherry, two flavors which are commonly used as targets for fantasy fragrances for lipstick perfumes.

As a sweetener, it modifies Anise and Anethole in licorice flavor compositions, and it is generally used in smaller amounts in many imitation fruit flavors for baked goods or hard candy, where heat stability is essential.

The normal concentration is about 10 to 30 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2672.

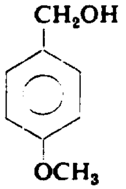
Prod.: from Anisaldehyde plus Acetone by condensation, followed by hydrogenation.

It can also be prepared from Methyl vinyl ketone by catalytic condensation with Phenol, followed by Methylation.

31-83; 68:752; 96-157; 103-266; 156-380;

## 249: ANISYL ALCOHOL

Anisalcohol.
Anisic alcohol.
*para*-Methoxy benzylalcohol.



$C_8H_{10}O_2 = 138.17$

Colorless liquid or opaque crystalline mass, melting at 25° C. Sp.Gr. 1.11-1.12. B.P. 259° C.

Insoluble in water, poorly soluble in Propylene glycol and Glycerin soluble in alcohol and oils.

Mild-floral, very sweet odor, reminiscent of Lilac and Vanilla with a faint, delicate, balsamic background.

Very useful in Lilac, Appleblossom, Sweet Pea, Gardenia, Jasmin, etc. Gives pleasant notes with Nitromusks and with certain types of non-Nitromusks. Good tenacity.

Finds some use in flavor compositions for imitation Chocolate, Cocoa, Fruit, Vanilla and in Licorice flavorings.

Concentrations are usually about 10 to 15 ppm, but could be higher since Anisyl alcohol is not a very powerful ingredient. It tends to produce "perfumey" notes at higher concentrations, however. The quality of Anisyl alcohol is extremely important for its use in flavors.

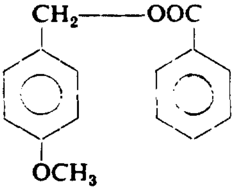
Prod. (many methods) e.g. from Anisaldehyde by catalytic hydrogenation. Consequently, the quality of the aldehyde monitors the quality of the alcohol.

G.R.A.S. F.E.M.A. No.2099.
FCC 1964-789.

5-63; 68-736; 90-491; 103-152; 103-266; 106-62; 140-130;

## 250: ANISYL BENZOATE

*para*-Methoxy benzylbenzoate.



$C_{15}H_{14}O_3 = 242.28$

Colorless viscous liquid.

Very faint, balsamic-floral odor of great tenacity. The odor quality varies considerably with the origin of the material.

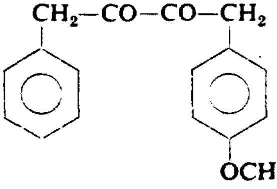
This ester is not frequently offered by the perfume industry.

It has been suggested as a fixative-blender for sweet florals, Oriental type fragrances, and in general as a blender with delicately sweet notes. However, it does not seem to contribute very unusual notes or effects, and may not ever become popular among the creative perfumers.

Prod. from Anisyl alcohol and Benzoic acid by direct esterification under azeotropic conditions in the presence of a catalyst.

86-14;

## 251: ANISYL BENZYL DIKETONE



$C_{17}H_{16}O_3 = 268.30$

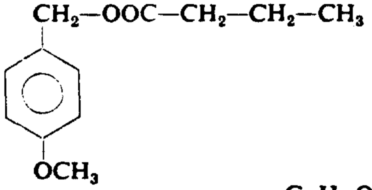
Reported as having a sweet "bitter Almond" and somewhat floral odor.

Very rarely offered from the usual manufacturers of perfume and flavor chemicals. Probably of little more than academic interest.

31-84;

## 252: ANISYL BUTYRATE

*para*-Methoxy benzyl butyrate.



$C_{12}H_{16}O_3 = 208.26$

Colorless liquid. B.P. approximately 270° C.

Mild floral, intensely sweet and warm-slightly fruity, Plum-like odor.

Occasionally used in perfumery as a fixative-modifier in fruity-floral fragrance types (Gardenia, Freesia, Magnolia, etc.).

Finds some use in flavor compositions for imitation Vanilla, in some fruit flavors and in Licorice flavorings.

Concentrations are usually about 10 to 14 ppm in the finished consumer product.

Prod. from Anisyl alcohol and *n*-Butyric acid by direct esterification under azeotropic conditions.

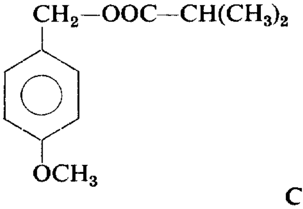
The *n*-butyrate seems to be slightly less stable than the *iso*-butyrate, and therefore often show an unpleasant "butyric" topnote due to traces of free acid.

G.R.A.S. F.E.M.A. No.2100.

86-14;

## 253: ANISYL iso-BUTYRATE

*para*-Methoxybenzyl-*iso*-butyrate.



$C_{12}H_{16}O_3$ = 208.26

Colorless liquid. Sp.Gr. 1.06.

Heavy-sweet, floral and mildly fruity odor. Somewhat fresher than the *n*-Butyrate, and not as "jam-like".

Finds some use in perfumery as a modifier-fixative for Lilac and other florals in which Anisyl alcohol and/or esters may be applied.

Used in flavor compositions for imitation fruit flavors, Peach, Plum, Cherry, Vanilla, etc.

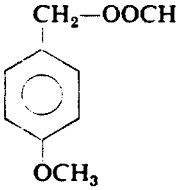
Prod. from Anisyl alcohol and *iso*-Butyric acid by direct esterification under azeotropic conditions.

(The *n*-Butyrate is included in the G.R.A.S. list in the U.S.A.).

3-11; 4-13;

## 254: ANISYL FORMATE

*para*-Methoxybenzyl formate.



$C_9H_{10}O_3$ = 166.18

Colorless liquid. Sp.Gr. 1.14.

Sweet herbaceous-green, yet somewhat dry odor with a faintly musty, but not unpleasant undertone. Reminiscent of Vanilla beans (cured) with an exotic-floral background, much drier than the acetate.

Sweet and slightly spicy-green Vanillabean-like taste.

Useful in perfumes for Lilac, Heliotrope, Jasmin, Ylang-Ylang, Tuberose, Gardenia, etc.

Finds extensive use in flavor compositions for imitation Raspberry, Blackberry, Black-currant, Strawberry, Vanilla, Fruit, and in Licorice flavorings, etc.

Concentrations are usually about 12 to 15 ppm in the finished product.

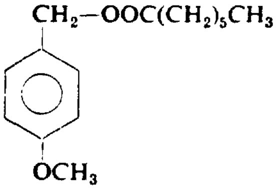
Prod. from Anisalcohol and Formic acid. The quality of the Anisalcohol is extremely important for the quality of Anisyl formate for flavors. Any trace of phenolic or cresylic odor can ruin the desirable flavor picture.

G.R.A.S. F.E.M.A. No.2101.

3-11; 4-12; 77-180; 86-14; 106-63; 155-88; 140-133;

## 255: ANISYL HEPTOATE

*para*-Methoxybenzyl heptanoate.



$C_{15}H_{22}O_3 = 250.34$

Colorless oily liquid.

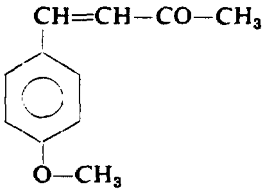
Very faint fruity odor, reminiscent of Peach juice or Apricot juice. Very tenacious, and this ester may under proper conditions of blending contribute pleasantly to a composition of lower boiling materials.

Suggested for use in Vanilla, Peach, Cherry, Apricot, etc.

Prod. from Anisyl alcohol and Heptanoic acid by direct esterification under azeotropic conditions.

## 256: ANISYLIDENE ACETONE

Methyl-*para*-methoxycinnamylketone.
*4*-(*para*-Methoxyphenyl)-*3*-buten-*2*-one.
*para*-Methoxybenzalacetone.
"Aldehyde Foin Coupe". (Haarmann & Reimer).
Anisal acetone.
*para*-Methoxy benzylidene acetone.
*para*-Methoxy methyl styrylketone.



$C_{11}H_{12}O_2 = 176.22$

White or yellowish leafy crystals. M.P. 74° C.

Insoluble in water, soluble in alcohol and oils.

Slightly pungent, but in dilution sweet, floral and creamy odor of considerable tenacity.

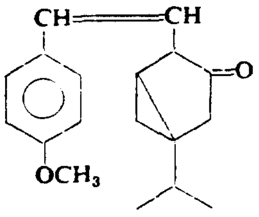
This ketone, like many related ketones, has met with much resistance from perfumers and dermatologists. However, it has survived all attacks under the usual and probably reasonable argument, that in normal concentrations it will have no harmful effects on the human skin. Undoubtedly, perfumers are using scores of materials with a much shorter history of successful application.

It finds use in many floral perfume compositions, mainly Cassie bases, Acacia, Lilac, Sweet Pea, Hyacinth, etc. In even lower concentration, it may give interesting effects in Lavender, Fougères, New Mown Hay (for which it was originally intended), etc.

Prod.: from Anisaldehyde and Acetone by condensation using diluted hydrochloric acid as condensing agent.

86-14; 26-414; 68-989; 86-88; 160-886; B-VIII-131;

## 257: ANISYLIDENE THUJONE



$C_{18}H_{22}O_2 = 270.37$

Yellowish oily liquid, solidifying in the cold.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet, fruity-herbaceous, Mimosa-Honey-like, tenacious odor.

This relatively rare perfume material is not offered commercially under its proper chemical name. It has been suggested for use in perfumes since the 1930's, and has never become a very famous material. However, this fact should not always be taken as indication that the material is uninteresting. It has managed to escape perhaps 9 out of every 10 perfume laboratories, and most perfumers never use it, many have never heard of it.

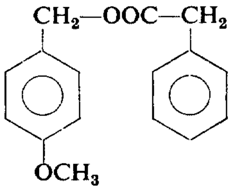
For special purposes, in the creation of unusual or "unconventional" bases, it has found some application.

Prod.: by condensation of Thujone with Anisaldehyde under mildly alkaline conditions.

See also: Cinnamylidene pulegone.

## 258: ANISYL PHENYLACETATE

*para*-Methoxy benzyl phenylacetate.



$C_{16}H_{16}O_3$ = 256.30

Colorless oily liquid.

Very faint balsamic-rosy odor of great tenacity. Less honeylike, more floral than Benzyl phenylacetate, also more fruity than this.

Occasionally used in perfumes as a blender-fixative, giving considerable "background" or "fond" in the composition.

Used in flavor compositions mainly as a modifier in Honey flavors, and occasionally as a fixative in flavors for baked goods, candy and other "heat-treated" consumer products.

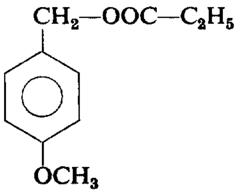
Concentrations are usually as low as 5-7 ppm.

G.R.A.S.

Prod. from Anisyl alcohol and Phenylacetic acid by direct esterification with a catalyst under azeotropic conditions.

## 259: ANISYL PROPIONATE

*para*-Methoxybenzyl propionate.



$C_{11}H_{14}O_3$ = 194.23

Colorless, slightly oily liquid.

Sp.Gr. 1.09. B.P. 277° C.

Insoluble in water, poorly soluble in Propylene Glycol, almost insoluble in Glycerin. Soluble in alcohol and oils.

Sweet fruity, floral and somewhat Vanilla-like odor.

Useful in mild, sweet floral fragrances: Lilac, Appleblossom, Sweet Pea, Magnolia, Peony, Acacia, Mimosa, etc. Blends excellently with the floral aldehydes.

Finds considerable use in flavor compositions for imitation Apricot, Cherry, Peach, Quince, Raspberry, and in Licorice flavorings.

Concentrations usually about 20 ppm.

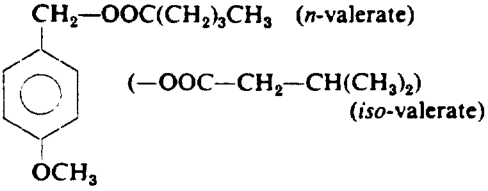
Prod. by direct esterification of Anisyl alcohol with Propionic acid or Propionic anhydride.

G.R.A.S. F.E.M.A. No.2102.

4-13; 86-14;

## 260: ANISYL VALERATE

*para*-Methoxybenzyl-*n*-pentanoate.
NOTE: Commercial product is most often: Anisyl *iso*-valerate.



$C_{13}H_{18}O_3 = 222.29$

Colorless liquid. B.P. approximately 282° C.

Very sweet, fruity-Apricot-Nectarine-Grenadine-like odor.

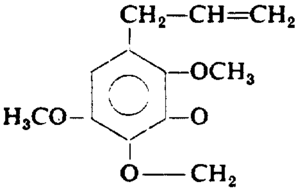
Probably not used in perfumery except in rare cases.

Interesting in flavor compositions for imitation Grenadine, Cherry, Apricot, etc.

Prod. from Anisyl alcohol and *n*-Valeric acid* by direct esterification under azeotropic conditions. (*or: *iso*-Valeric acid).

## 261: APIOLE

"Parsley Apiole".
*1*-Allyl-*2,5*-dimethoxy-*3,4*-methylene dioxybenzene.



$C_{12}H_{14}O_4 = 222.24$

Colorless crystal needles. M.P. 30° C. Once liquefied, this material may remain supercooled for a considerable length of time.
B.P. 298° C. Sp.Gr. 1.17 (liquid). Insoluble in water, soluble in alcohol and oils.

Faint, herbaceous-warm, Parsley-like odor.

Rather sharp, burning-herbaceous taste.

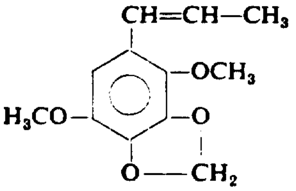
As a chief constituent of the essential oil from a very popular condiment, this chemical has some significance. However, it has not gained much popularity as such in flavor compositions. In most countries, it is NOT permitted for use in food flavorings. With respect to toxicity, it can be classified ad moderately toxic. 25-35 grams may kill an adult man. This degree of toxicity is much lower than that of many chemicals permitted for food use.

Prod.:
1) by isolation from Parsley seed oil, containing 70-80% Apiole.
2) synth. from *2*-Hydroxy-*3,4*-methylenedioxy-*1*-allyl benzene by oxidation followed by methylation.

68-978; 72-92; 85-28; 86-13; 90-485; 100-93; 104-507;

## 262: iso-APIOLE

*1*-(*1*$^2$-Propen-*1*-yl)-*2,5*-dimethoxy-*3,4*-methylenedioxybenzene.



$C_{12}H_{14}O_4 = 222.24$

Crystals. M.P. 55-56° C. B.P. 304° C.

Warm-herbaceous, more resinous-earthy than Apiole. Less Parsley-like.

See notes under Apiole.

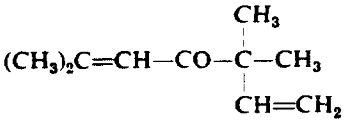
*iso*-Apiole is formed from Apiole.

NOTE: Another isomer is Dill apiole (see under that name).

68-979; 72-91; 90-486;

## 263: ARTEMISIA KETONE

*2,5,5*-Trimethyl heptadien-*2,6*-one-*4*.



$(CH_3)_2C{=}CH{-}CO{-}\underset{CH{=}CH_2}{\overset{CH_3}{C}}{-}CH_3$

$C_{10}H_{16}O = 152.24$

Pale yellowish liquid. B.P. 182° C. Sp.Gr. 0.89.

Green-herbaceous odor, at the same time warm and minty, slightly bitter-woody.

Has been suggested for use in perfumery to introduce new and interesting herbaceous notes, particularly for Men's fragrances, new versions of Fougere, etc.

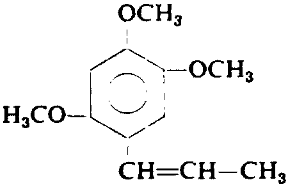
However, this ketone is in poor supply so far, and it is doubtful whether this situation will improve considerably.

Prod. from the essential oil of Artemisia annua by isolation.

89-193; 65-386;

## 264: ASARONE

*1,2,4*-Trimethoxy-*5*-propenylbenzene. Exists in *alpha*- and *beta*-forms.



$C_{12}H_{16}O_3 = 208.26$

Colorless cryst. M.P. 66-67° C. B.P. 296° C.

Pure Asarone is reported to be virtually odorless and tasteless. However, available samples of the material have in experiments shown perceptible influence upon the odor of compositions containing lower boiling perfume materials.

Insoluble in water, soluble in alcohol and oils.

The material has been suggested for use as a fixative-blender with Patchouli-like odor character.

Prod.

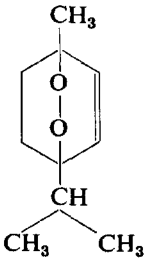
1) by isolation from the essential oil of Acorus Calamus.
2) synth. by reduction of Asaraldehyde.

68-978; 85-29; 90-477; 100-105;

## 265: ASCARIDOLE

*1*-Methyl-*4*-*iso*-propyl cyclohexene-*2*-dioxide-*1,4*.

*1,4*-Peroxido-*para*-menthene-*2*.



$C_{10}H_{16}O_2 = 168.24$

Pale yellowish oil. Sp.Gr. 1.01. Solidifies in the cold, melts at 2-3° C.

Insoluble in water, soluble in alcohol and oils.

Nauseating "headachy" odor, choking-herbaceous, minty undertone, unpleasant taste.

This material is mainly included for completion, and for the hazard it presents. Being the chief constituent of Worm*seed* oil which is produced - among other places - in the Midwestern States of the U.S.A. - it presents a hazard of confusion with Worm*wood* oil - also produced in the Midwest U.S.A., and used in perfumes and (previously) in flavors.

The two oils have no major constituents in common and the botanicals from which they are made are not closely related.

Ascaridole: HAZARD:

1) May cause fire if heated or if brought in contact with acids. Distil under vacuum only.
2) Toxicity: 5 grams may kill a child.

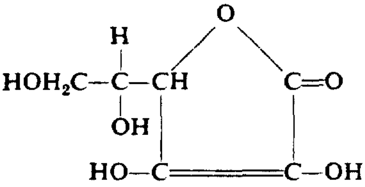
Prod.

1) By isolation from Chenopodium oil (Wormseed oil).
2) Synth. from *alpha*-Terpinene by oxidation.

67-534; 85-29; 90-723; 100-105;

## 266: ASCORBIC ACID

*laevo*-Ascorbic acid.
Vitamin C.
L-*3*-Ketothreohexuronic acid, lactone.
L-Xyloascorbic acid.



$C_6H_8O_6 = 176.13$

White crystal plates or needles. M.P. 192° C.

25% soluble in water. 3% soluble in alcohol. Insoluble in oils. 5% soluble in Propylene glycol.

Dry Ascorbic acid is virtually odorless.

Rather sharp, but pleasant acid taste. The material is NOT stable in aqueous solution. The solution is easily oxidized.

Ascorbic acid is useful as

1) an Antioxidant (keeps fruits and vegetables from discoloring during processing.
2) a Vitamin*).
3) an acid-modifier in certain flavors and foods.

Concentrations permissible up to 6000 (six thousand) ppm in candy. This is equivalent to one part per 160 parts of functional product.

G.R.A.S. F.E.M.A. No.2109.

Prod from D-Glucose via D-Sorbitol to L-Sorbose, followed by carboxylation and acid hydrolysis.

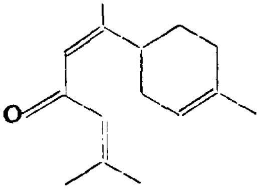
66-1276; 100-106; 1-743; 1-744; 140-145;

See also Erythorbic acid (= *iso*-Ascorbic acid).

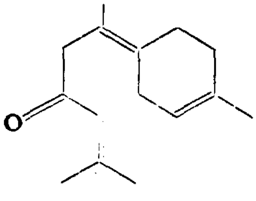
*) According to international pharmaceutical standards, one unit of Vitamin C is the activity derived from 0.05 mg Ascorbic acid.

## 267: ATLANTONE

Exists as *alpha*- and *gamma*-Atlantone:



*alpha*-Atlantone



*gamma*-Atlantone

$C_{15}H_{22}O = 218.34$

Viscous, pale yellowish or almost colorless liquid. (Commercial product not well-defined). B.P. approximately 282° C. Sp.Gr. 0.96.

Woody-animal, rather powerful odor with pleasant sweet background.

Has been suggested as a modifier-substitute for East Indian Sandalwood oil or Santalol. However, it presents quite different tonalities and should be considered a perfume material of unique character.

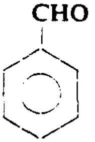
Its availability has fluctuated with the uneven supply of Moroccan (Atlas) Cedarwood oil, and the ketone is only rarely available.

Prod. by isolation from Atlas Cedarwood oil, or from Himalayan Deodar Cedarwood oil, after boration of the heart fractions of the vacuumdistilled oil.

67-695; 89-415; 65-448/449;

## 268: BENZALDEHYDE

"Amandol". (Rhone-Poulenc).
"Amandiol" (Lautier Fils).
Benzene carbonal.
Benzene methylal.
Benzoic aldehyde.
"Bitter Almond oil, synthetic".



$C_7H_6O = 106.12$

Colorless liquid, soluble 0.3% in water. Soluble in alcohol and oils. Sp.Gr. 1.05.
B.P. 179° C.

Powerful sweet odor, reminiscent of freshly crushed bitter Almonds. Burning, but sweet taste in proper dilution.

Sometimes used in perfumery for special topnote effects, and as a trace component in certain floral compositions (Lilac, Sweet Pea, etc.).

Extensively used in flavor compositions, not only in "Almond" flavors, but also in imitation Berry, Butter, Apricot, Brandy, Cherry, Coconut, Liquor, Peach, Plum, Pecan, Pistacio, Rum, Spice, Vanilla, etc.

It forms the major if not the only flavor component in "Marcipan" candy (ground sweet Almond kernels with a few bitter Almond kernels in).

Concentrations usually around 150 to 160 ppm in the finished product, except in chewing gum, where concentrations up to 800 ppm are used.

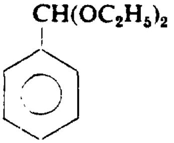
G.R.A.S. F.E.M.A. No.2127.

Prod.

1) by oxidation of Toluene.
2) from Benzylidene chloride, made from Toluene.
3) from Benzyl alcohol made from Benzyl chloride.

4-19; 5-103; 77-20; 77-204; 85-32; 100-128; 106-65; 156-48; 140-161; 85-32;

## 269: BENZALDEHYDE DIETHYLACETAL



$C_{11}H_{16}O_2 = 180.15$

Colorless liquid. Sp.Gr. 0.98.

Soluble in alcohol and oils.

Sweet and mild, green odor, faintly reminiscent of the odor of Bitter Almond, but more herbaceous.

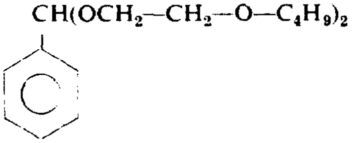
Has been suggested for use in perfumes because it is more stable to alkali than the aldehyde. However, it does not lend the power or the character of the free aldehyde.

In flavors it offers some advantage in being milder, easier to handle, but it must be kept in mind that - like most other acetals - this material is sensitive to mild acid, a condition prevalent in many functional products containing artificial flavor (yet most Nut-flavors end up in neutral media, not acid).

Prod. from Benzaldehyde and Ethylalcohol.

86-21;

## 270: BENZALDEHYDE-DI-(ETHYLENEGLYCOL MONOBUTYLETHER)-ACETAL



$C_{19}H_{32}O_4 = 324.47$

Colorless or very pale straw-colored oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

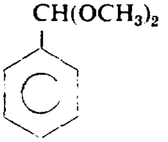
Mild-herbaceous, sweet and floral odor. The odor varies considerably with the age of the material; and samples from different suppliers have shown quite different odor characteristics. It is conceivable that the commercial material – rarely offered under its proper name – is not a well-defined, single chemical.

This acetal was developed many decades ago, after the discovery of interesting odors in simple cyclic acetals of aromatic aldehydes. The Ethyleneglycol acetal of Phenylacetaldehyde was for a long time considered to be of substantial interest, professionally and academically to the perfumers and chemists, but it has lost most of its importance.

The title acetal will lend some of the more valuable and interesting parts of the Jasmin fragrance, some of the herbaceous notes which cannot be supplied by Amylcinnamic aldehyde, but the acetal lacks the power and versatility of ACA.

Prod.: by condensation of Benzaldehyde with Ethyleneglycol monobutylether, commercially known as "Butyl cellosolve".

## 271: BENZALDEHYDE DIMETHYLACETAL



$C_9H_{12}O_2 = 152.20$

Colorless liquid. Sp.Gr. 1.03. B.P.198° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Sweet-green and warm odor, remotely reminiscent of Nuts and Bitter Almonds.

Occasionally used in perfumes for special effects such as green-floral topnotes in Lily or Narcisse bases.

Used in flavor compositions for imitation Cherry, Fruit, Nut, Almond, etc.

Concentration usually up to 60 ppm in the finished product. It should be remembered that the acetal is sensitive to mild acid and will not be stable in finished products of low pH.

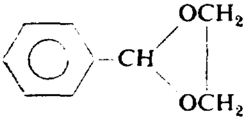
Prod. from Benzaldehyde and Methylalcohol.

G.R.A.S. F.E.M.A. No.2128.

4-19; 86-21;

## 272: BENZALDEHYDE ETHYLENEGLYCOLACETAL

*2*-Phenyl-*1*,*3*-dioxolane.



$C_9H_{10}O_2 = 150.18$

Colorless viscous liquid.

Almost odorless when free from Benzaldehyde, but traces of moisture will free some aldehyde and influence the odor.

Suggested for use in flavor compositions where storage conditions favor a more stable form of Benzaldehyde.

The aldehyde is liberated under influence of Water, Heat or Acid, all of which conditions are frequently occurring in the functional products containing artificial flavor.

Since Ethylene glycol is considered slightly toxic and banned from food use in many countries, the Glyceryl acetal is favored more generally for the above purposes. (See next).

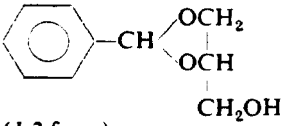
Prod. from Benzaldehyde and Ethylene glycol by condensation.

See also: Formaldehyde
phenylethyleneglycolacetal.

## 273: BENZALDEHYDE GLYCERYL ACETAL

"Benzalglycerin"
Benzaldehyde cyclic acetal of Glycerin.
Benzylidene glycerol (*1*,*2*- and *1*,*3*-).
*4*-Hydroxymethyl-*2*-phenyl-*meta*-dioxolane, and: *5*-Hydroxy-*2*-phenyl-*1*,*3*-dioxane.
The commercial product is a mixture of two acetals:

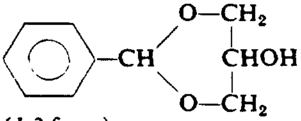
60% of this:



(*1*,*2*-form)

$C_{10}H_{12}O_3 = 180.20$

and 40% of this:



(*1*,*3*-form)

$C_{10}H_{12}O_3 = 180.20$

Colorless viscous liquid. B.P. approximately 280° C. Sp.Gr. 1.19.

Used in flavor compositions where lower volatility and improved stability towards air (oxygen) is desirable, and Benzaldehyde as such seems too volatile and unstable.

The acetal will liberate Benzaldehyde under influence of heat, water or mild acid, conditions which frequently exist in functional products containing artificial flavor.

The acetal itself has a very faint odor, barely reminiscent of Bitter Almond. Soluble in alcohol and oils.

Used in fruit flavors, imitation Almond, Cherry, Nut, etc. in concentrations equal to 100 ppm in the finished consumer product.

Chewing gum may contain up to 800 ppm of the acetal. Chewing gum is the most common outlet for this acetal.

G.R.A.S. F.E.M.A. No.2129.

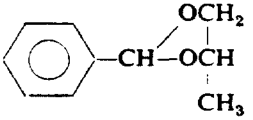
Prod. from Benzaldehyde and Glycerin by condensation, using Phosphoric acid as a catalyst, and making use of azeotropic distillation to remove reaction water.

Also by heating Glycerol and Benzaldehyde in $CO_2$ atmosphere to 150° C. The *1*,*3*-isomer is crystallizable and may be separated.

107-164; 66-1031; 161-187;

## 274: BENZALDEHYDE PROPYLENEGLYCOL ACETAL

*4*-Methyl-*2*-phenyl-*meta*-dioxolane.



$C_{10}H_{12}O_2 = 164.20$

Colorless viscous liquid. Soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Used in flavor compositions for imitation Cherry, Almond, Nut, etc. particularly where greater stability and lower volatility of the "Bitter Almond"-theme is desirable.

The acetal itself is practically odorless but will liberate Benzaldehyde under influence of moisture (particularly in the presence of acid) and heat.

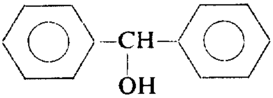
See also previous monograph.

G.R.A.S. F.E.M.A. No.2130.

Prod. by condensation of Benzaldehyde with Propylene glycol. The reaction water is removed in Bidwell trap (azeotropic setup).

## 275: BENZHYDROL

Diphenyl carbinol.



$C_{13}H_{12}O = 184.24$

White or colorless crystals. M.P. 69° C. B.P. 281° C.

Practically insoluble in water, soluble in alcohol, miscible with oils.

The crystals have a very faint musty-rosy odor, somewhat similar to that of Benzophenone and Trichloromethyl phenyl carbinyl acetate.

In actual use, the odor is more perceptible, and the material does have some fixative effect. However, it does not seem to offer any advantages over Benzophenone (from which it is most conveniently prepared).

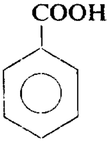
In the author's opinion, this material has little, if any, use in perfumes or flavors.

Prod.: by reduction of Benzophenone, e.g. with zinc in aqueous alkali.

37-513; 68-1059;

## 276: BENZOIC ACID

Benzenecarboxylic acid.
Phenylformic acid.
Dracylic acid (old name).



$C_7H_6O_2 = 122.12$

White crystal plates or leaflets, or needles.

Odorless when pure. However, the commercial product usually carries a peculiar, unpleasant "Urine-like" or faint Carbylamine-like odor, which is hardly perceptible unless a large quantity of the acid is smelled (fibre-drums or larger quantities).

M.P. 122° C. B.P. 249° C. Volatile with steam. Sublimes above 100° C.

0.35% soluble in water, 5% soluble in boiling water, 33% in alcohol. Soluble in most perfume materials.

The acid finds use as a preservative (as acid or its sodium salt) in fruit juices, beverages, etc.

It is used in Chocolate, Lemon-, Orange-, Cherry-, Fruit- and Nut preserves and in Tobacco products. Concentrations amount to 250 ppm in the finished product. The same concentration is used in icings.

Prod.

1) from Phthalic anhydride (various methods)
2) from Toluene by oxidation.

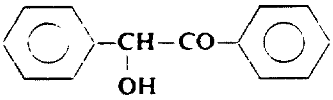
G.R.A.S. F.E.M.A. No.2131.

26-424; 68-543; 100-133; B-IX-92; 140-149;

## 277: BENZOIN

*2*-Hydroxy-*2*-phenylacetophenone.
*dl*-Benzoyl phenylcarbinol.

Note: Do not confuse this chemical with the crude botanical of same name. (Gum)Benzoin, see: S. Arctander: "Perfume and Flavor Materials of Natural Origin", 1960. Page 87.



$C_{14}H_{12}O_2 = 212.24$

White crystals. M.P. 137° C. B.P. 344° C. Slightly soluble in hot water. Slightly soluble in alcohol and oils.

Very faint, sweet, nondescript odor.

Suggested for use (and actually used) in imitation Butter flavors, Butterscotch, Fruit, Liquor, Vanilla, etc. and in imitation Rum flavors.

Concentration up to 5 ppm in the finished product.

(The author questions the effect at this use level).

This chemical is used mainly in beverages (at concentrations about 5 ppm), but the actual extension of use is very small.

The author suspects again here a confusion (see also ANISOLE) in this case with (Gum) Benzoin. Once the error has been recorded it may have been psychologically repeated through many decades, and only rarely investigated. The use of NATURAL (Gum) BENZOIN in all the above flavor types is very conceivable.

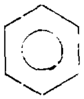
G.R.A.S. F.E.M.A. No.2132.

Prod. from Benzaldehyde in alcoholic solution with Sodium cyanide.

26-424; 68-1168; 100-133; B-VIII-166;

## 278: BENZOL

Benzene.
Cyclohexatriene.



$C_6H_6 = 78.11$

Colorless mobile liquid. B.P. 80° C. Sp.Gr. 0.88.

Solidifies in the cold, melts at 5°,5 C.

0.2 pct. soluble in water, miscible with absolute alcohol and oils.

This chemical is included only because it is used widely as a solvent in extracting aromatic substances from crude botanical materials for use in perfumes (and occasionally in flavors). Many perfume extracts therefore contain traces of this solvent.

Characteristic "gassy" hydrocarbon odor, choking, diffusive, warm.

HAZARDS:

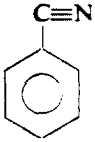
1) Flashpoint 11° C. - vapors explosive in air mixture.
2) Skin-penetrating - toxic.
3) Inhalation - toxic. Concentrations above 100 ppm. in air may cause death to human beings.

Produced from coal (gas).

26-420; 100-129; 68-100; B-V-179;

## 279: BENZONITRILE

Phenyl cyanide.
Benzoic acid, nitrile.
Cyanbenzol.



$C_7H_5N = 103.12$

Colorless liquid. B.P. 190°.7 C. Sp.Gr. 1.01.

Insoluble in cold water. 1% soluble in boiling water. Miscible with alcohol and oils, but not soluble in liquid paraffin. Poorly soluble in Propylene glycol.

Recommended as a stabilizer for Benzaldehyde in industrial perfumes. The producer claims that one percent Benzonitrile added to Benzaldehyde acts as an Antioxidant upon the Aldehyde.

Discolors in the presence of iron. Unstable in the presence of acid, particularly if water is present.

This chemical is comparatively new on the market, and it may take some thorough testing before it can be firmly recommended for use in perfumes in general. So far, it would be interesting to use as a stabilizer for industrial perfumes, where conditions often cause a breakdown of Benzaldehyde quickly. The Nitrile is offered at about the same price as the technical grade Aldehyde.

TOXICITY: equal to that of Ammonia.

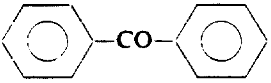
Prod. (many methods), e.g. from Aniline by diazoreaction.

1-530; 68-560;

info: Velsicol Corporation, Division of Tensyn,
Chattanooga, Tennessee, U.S.A.
Data sheet No.8163, March 1967.
Technical data bulletin, Nov. 1967.

## 280: BENZOPHENONE

Diphenyl ketone.
Benzoyl benzene.
(*alpha-*, *beta-*, *gamma-* and *delta*-forms are known).
Commercial (stable) form is: *alpha*-Benzophenone.



$C_{13}H_{10}O = 182.22$

White rhombic crystals or amorphous flakes. M.P. 48° C. (*alpha-*). B.P. 306° C.

Insoluble in Water and Glycerin, slightly soluble in Propylene glycol, 6% soluble in alcohol, soluble in most perfume oils.

Very faint, powdery-rosy, geranium-like odor with a slightly metallic note.

Used extensively in perfumes for sweet-woody-geranium-like notes in low-cost fragrances, soap perfumes, etc. Useful as a fixative. It has an extremely low vapor pressure at room temperature, and its effect upon the fragrance is only perceptible and apparent in mixtures with lower boiling items or at higher temperatures.

Occasionally used in flavors for imitation Apricot, Berry, Butter, Fruit, Nut, Peach, Vanilla, etc.

Concentration is usually traces only (a few ppm in finished product).

G.R.A.S. F.E.M.A. No.2134.
FCC 1964 page 791.

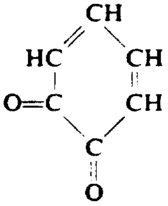
Prod. (many methods):

1) From Benzylchloride plus Benzol (condens.).
2) From Benzonitrile plus Phenyl Magnesium bromide.
3) By oxidation of Diphenylmethane with chromic acid.
   etc.

26-424; 30-250; 30-358; 68-1063; 86-21; 103-271; 106-67; 156-153; B-VII-410;

## 281: BENZOQUINONE

*ortho*-Benzoquinone.
Quinone.
*1,2*-Cyclohexadienedione.



$C_6H_4O_2 = 108.09$

Reddish prismatic crystals, M.P. 60-70° (decompos.)

Insoluble in water, soluble in Acetone, slightly soluble in oils.

Powerful, but relatively sweet buttery-Iodine-like odor.

The author doubts that this chemical is actually used in perfumes, but it is occasionally referred to as the type of odor found in certain other perfume chemicals.

Benzoquinone is occasionally referred to as being odorless (other sources).

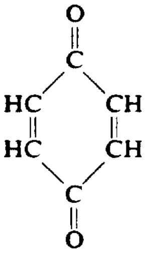
Among its drawbacks are the intense color, and the poor solubility.

Prod. from Catechol by oxidation.

26-672; 68-690; B-VII-600;

## 282: para-BENZOQUINONE

*para*-Quinone.
*1,4*-Cyclohexadiene-dione.



$C_6H_4O_2 = 108.09$

Yellowish monoclinic crystals. M.P. 116° C.
Sp.Gr. 1.32.

Almost insoluble in water, soluble in oils and alcohol.

Penetrating Chlorine-Iodine-like odor, pungent, "medicinal". The vapors are irritating to human mucous membranes and eyes.

Note: This material is modestly toxic: 10 grams may kill an adult man.

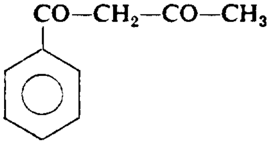
Probably not used as such in perfumes (not at all in flavors), but is occasionally mentioned as the prototype for "Quinone"-like odor.

Prod. from Aniline by oxidation with Dichromate, or by oxidation of Hydroquinone.

1-585; 26-672; 30-251; 68-691; 100-894; B-VII-609;

## 283: BENZOYL ACETONE

*4*-Phenylbutan-*2,4*-dione.
*omega*-Acetyl acetophenone.



$C_{10}H_{10}O_2 = 162.18$

White prismatic crystals. M.P. 61° C.
B.P. 261° C. Sp.Gr. (liquid) = 1.09.

Soluble in hot water, soluble in cold alcohol and oils.

Faint, but very tenacious balsamic-sweet, Vanilla-like odor of "Oriental" fragrance type. Also described as Tolu-balsam-like.

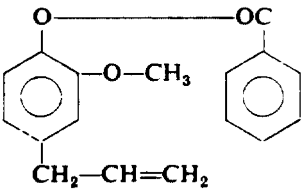
Used in perfume compositions for Oriental fragrances, Ambre bases, Leather bases, etc.

Prod. from Acetophenone plus Ethylacetate plus Sodium ethoxide, or directly by Acetylation of Acetophenone.

5-164; 26-426; 31-84; 86-22; B-VII-680;

## 284: BENZOYL EUGENOL

(Do not confuse with Benzyl eugenol).
Eugenol benzoate.
*4*-Allyl-*2*-methoxy phenylbenzoate.
Eugenyl benzoate.



$C_{17}H_{16}O_3 = 268.32$

White or almost white crystalline powder or colorless crystals. M.P. 70° C.
B.P. 360° C.

Insoluble in water, soluble in hot alcohol and many oils, but poorly soluble in cold alcohol.

Very mild balsamic-spicy odor of great tenacity and warm undertones. The spicy notes are more pronounced in older material. Freshly prepared material may be almost odorless.

This material finds a little use in perfume compositions, but its poor solubility is a disadvantage. Of the related materials, it seems that Benzyl-*iso*-eugenol is the one which has caught the most attraction to perfumers.

Eugenol benzoate finds some use in flavor compositions, e.g. various spice and fruit complexes. Its low rate of evaporation makes it suitable for fixation in flavors for baked goods, etc.

Concentration is usually about 10 ppm in the finished product.

Prod.: from Benzoyl chloride and Eugenol-sodium.

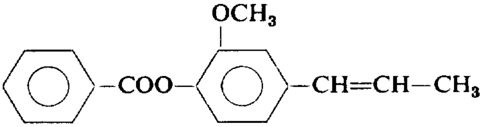
G.R.A.S. F.E.M.A. No.2471.

86-51; 90-438; 100-440; B-IX-135; 90-576;

## 285: BENZOYL-iso-EUGENOL

*iso*-Eugenol benzoate.

Note: Do not confuse with Benzyl-*iso*-eugenol.



$C_{17}H_{16}O_3$ = 268.30

White crystals.

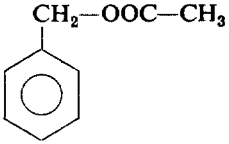
Insoluble in water, poorly soluble in cold alcohol, soluble in most perfume oils at normal use concentration.

Very faint, balsamic-sweet odor, usually carrying a trace of Vanillin-like odor.

Has been suggested for use in perfumery as a fixative and blender for mild florals, Carnation-type fragrances, Violet, etc. However, the relatively high cost of this material is almost prohibitive for its more extensive use.

Note: the Benzyl ether of *iso*-Eugenol = Benzyl-*iso*-eugenol, is generally used for the above perfumery purposes.

## 286: BENZYL ACETATE



$C_8H_{10}O_2$ = 150.17

Colorless mobile liquid. Sp.Gr. 1.06.
B.P. 215° C.

Practically insoluble in water and Glycerin. Soluble in alcohol and perfume oils. Slightly soluble in Propylene glycol.

Powerful but "thin", sweet floral, fresh and light, fruity odor reminiscent of Jasmin, Gardenia, Muguet, Lily and other flowers. Poor tenacity.

Very extensively used in perfumery, from the lowest priced industrial odors to the most highly appreciated cosmetic fragrances, often constituting the main ingredient in a perfume oil. It is almost inevitably the largest component in Jasmin and Gardenia fragrances, and it enters in a multitude of other floral fragrance types in smaller proportions. Its poor tenacity is usually compensated for by proper blending with higher esters of Benzyl alcohol, and with suitable fixatives. In the industrial odors, the volatility of Benzyl-acetate is often only an advantage.

Frequently used in flavor compositions, for imitation Apple, Apricot, Banana, Butter, Cherry, Peach, Pear, Plum, Pineapple, Quince, Raspberry, Strawberry, Violet, etc. etc.

Concentration usually about 35 ppm, except in chewing gum where it may be as much as 800 ppm.

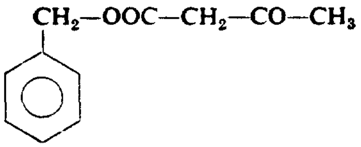
Prod. from Benzyl chloride and Potassium acetate in presence of a catalyst.

G.R.A.S. F.E.M.A. No.2135.
FCC 1964-793.

4-20; 106-68; 156-58; 26-428; B-VI-435; 100-137; 85-33 (toxicity); 103-94; 5-260; 90-328; 77-183; 140-136;

## 287: BENZYL ACETO ACETATE

*2*-Propanone carboxylic acid, Benzylester.
Benzyl acetyl acetate.
NOTE: Do not confuse with Benzyl acetoacetic ester, which is: Ethyl benzyl aceto acetate.



$C_{11}H_{12}O_3 = 192.22$

Colorless liquid.

Pleasant balsamic-herbaceous and fruity odor, suggestive of "Oriental" fragrances, Ambre, etc.

Occasionally used in perfumery for special notes. Blends very well with refined Labdanum extracts, *iso*-Butyl cinnamate, Ionones, etc. and lends a natural, mellow topnote to woody-floral or herbaceous-floral fragrances. Although relatively high boiling, it appears in a fragrance at the very initial notes with surprising tenacity.

Also used in flavor compositions, mainly in Berry and Fruit flavors in concentrations equal to 50 ppm in the functional consumer product.

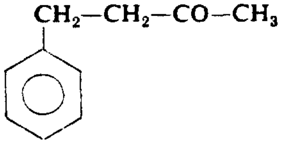
G.R.A.S. F.E.M.A. No.2136.

Prod. from Benzyl alcohol, Sodium metal and Ethyl acetate.

4-20;

## 288: BENZYL ACETONE

*4*-Phenylbutan-*2*-one.
"Jasmarol".
*beta*-Phenylethyl methyl ketone.
Methyl-phenylethyl ketone.



$C_{10}H_{12}O = 148.21$

Colorless liquid. Sp.Gr. 0.99. B.P. 235° C.

Insoluble in water, soluble in alcohol and oils.

Floral-green odor, fresher than that of Benzylacetate, more lasting. Stable in soap.

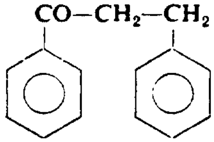
Suggested for use in perfumes as a modifier for Benzylacetate, particularly in soap fragrances. Its somewhat sharper character can at times be an advantage for the more robust job of perfuming a soap.

Prod. (many methods), e.g. by Claisen condensation of Benzaldehyde and Acetone, followed by hydrogenation of the formed Benzylidene acetone.

4-20; 5-162; 86-22;

## 289: BENZYL ACETOPHENONE

Dihydro chalkone.
*1,3*-Diphenylpropan-*1*-one.



$C_{15}H_{14}O = 215.32$

White crystals or crystalline powder or flakes. M.P. 73° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild and sweet, balsamic-floral odor of excellent tenacity.

This ketone, rarely offered commercially, finds some use in perfume compositions as a fixative and modifier in herbaceous-floral or woody-rosy fragrance types. It is a good fixative for Lavender and Fougere, but it does not contribute much odor, except a sweet, creamy-balsamic undertone, which is often quite desirable. It blends well with Ylang-Ylang, Labdanum, Ionones, etc. and it is stable under normal alkaline conditions in finished products.

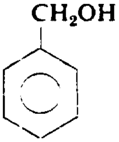
Prod.:

1) by catalytic reduction of Benzylidene acetophenone over Platinum oxide in Ethylacetate.
2) by oxidation of the corresponding alcohol (Phenyl-Phenylethylcarbinol) with Chromic acid.

68-1171;
see also: Benzylidene acetophenone (monograph).

## 290: BENZYL ALCOHOL

Phenyl carbinol.
Phenyl methanol.
*alpha*-Hydroxytoluene.



$C_7H_8O = 108.14$

Colorless liquid. Sp.Gr. 1.05. B.P. 205° C.

Soluble 4 % in water, miscible with alcohol and oils.

Faint, nondescript odor, rather sweet, but varies considerably with the quality of the alcohol.

The taste (in water) is rather sharp, chemical, nondescript, and the impurities will usually show up very conspicuously in water solution of Benzyl alcohol.

Used in perfumery as a blender, in some florals quite extensively. Jasmin, Gardenia and Lilac may often be composed using Benzyl alcohol although this material is really dispensable in most cases.

Used frequently in flavor compositions: in imitation Blueberry, Cherry, Grape, Honey, Loganberry, Muscatel, Nut, Orange, Raspberry, Vanilla, Walnut, and in Floral type flavors, Fruity types, Liquor types, Rootbeer, Rose, Violet, etc.

Concentrations may amount to 220 ppm in the finished product, or as high as 1200 ppm in chewing gum.

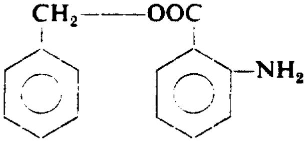
Prod. from Benzyl chloride and Potassium (or Sodium) carbonate.

G.R.A.S. F.E.M.A. No.2137.

4-21; 100-137; 103-126; 106-69; 26-428; 156-55; B-VI-428; 140-129;

## 291: BENZYL ANTHRANILATE

Benzyl-*ortho*-aminobenzoate.



$C_{14}H_{13}NO_2 = 227.27$

Colorless oily liquid. B.P. 315° C.
Sp.Gr. 1.16.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Faint, but pleasant floral-citrusy odor, as always depending upon the quality of the ester, and the method of preparation.

It has been suggested for use in Citrus fragrances as a "Grapefruit" type modifier, and generally as a modifier for other citrus odors. Its low vapor pressure makes it an excellent fixative for the more volatile citrus materials.

Certain floral fragrances can benefit from this particular note: Lily, Freesia, etc.

Prod.: (many methods):

1) From Methyl anthranilate and Benzyl alcohol (Trans-esterification).

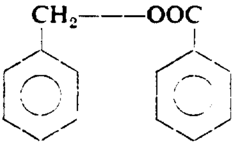
2) From Methyl anthranilate and Benzyl acetate (Cross-esterification).
3) From Phthalimide and Sodium hydroxide solution plus Benzyl alcohol, then treatment with Sodium hypochlorite.
4) From Isatoic anhydride and Benzyl alcohol.

The latter method is said to produce the highest perfumery quality ester.

86-22;

## 292: BENZYL BENZOATE

Benzyl benzene carboxylate.
Benzyl phenyl formate.
Spasmodin.
Ascabiol.
Benylate.
(and many other names, particularly pharmaceutical tradenames).



$C_{14}H_{12}O_2 = 212.25$

Colorless oily liquid. B.P. 324° C. Sp.Gr. 1.12.

Solidifies in the cold, melts at 21° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Faint, sweet-balsamic odor, floral undertone. Trace impurities may ruin the odor picture from a perfumery point of view.

A classic fixative-blender and solvent in perfumes. Also a modifier in heavier florals, Oriental type fragrances, etc., Tuberose, Ylang-Ylang, Lily, Gardenia, etc. Largely substituted by Benzyl salicylate when a faint odor is desirable. As a solvent for Nitromusks, Benzylbenzoate can not compete with Diethyl phthalate in cost, and the practise of keeping Nitromusks in solution on the perfumer's shelf is, in the author's opinion, outdated.

Benzyl benzoate is used in flavor compositions – partly as a fixative – e.g. imitation Cheese, Cherry, Liquor, Loganberry, Muscatel, Nut, Rum, Pineapple, Strawberry, etc.

Concentrations are usually about 40 ppm in the finished product, but may be as high as 300 ppm in chewing gum.

NOTE: Benzyl benzoate seems to have a specifically high toxicity towards certain animals, in no proportion to the comparatively low toxicity to human beings.

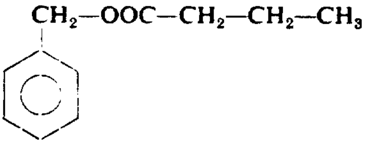
G.R.A.S. F.E.M.A. No.2138.

Prod. from Sodium benzoate and Benzyl chloride, sometimes using Triethylamine as a catalyst.

4-21; 5-257; 85-34 (toxicity); 100-137; 103-129; 106-70; 156-60;

## 293: BENZYL BUTYRATE

Benzyl-*n*-butyrate.
Benzyl-*n*-butanoate.
"Aldehyde C-19" (so-called).



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. B.P. 240° C. Sp.Gr. 1.01.

Insoluble in water, Propylene glycol and Glycerin, soluble in alcohol and oils.

Heavy, fruity-floral odor, mainly fruity, like Plum.

Used in perfume compositions as a modifier-companion to Benzyl acetate and or Benzyl propionate. Performs well in soap. Also as a modifier for floral-fruity notes in Acacia, Geranium, Muguet, Rose, Lily, etc. Must be used in concentrations far below those of Benzyl acetate.

In flavor compositions the ester is used for imitation Apricot, Butter, Cheese, Liquor, Loganberry, Muscatel, Nut, Peach, Pear, Raspberry, Strawberry, Pineapple, etc. Also suggested for Mango imitation flavor.

Concentrations are usually as low as 10 ppm, but may be up to 350 ppm in chewing gum.

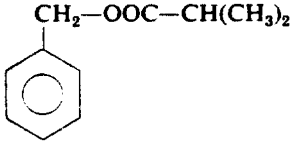
Prod. from *n*-Butyric acid and Benzyl alcohol by direct esterification using azeotropic conditions.

G.R.A.S. F.E.M.A. No.2140.
FCC 1964-795.

4-21; 5-233; 103-114; 106-71; 156-60;

## **294: BENZYL**-iso-**BUTYRATE**

Benzyl-*2*-methylpropanoate.
"Pineapple Aldehyde C-19" (old name for a specialty mainly consisting of this ester).



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Sp.Gr. 1.01.

Fruity-floral odor, somewhat fresher than that of the *n*-Butyrate, not as heavy. Relatively powerful, floral-fruity, berry-like taste.

Useful in fruity-spicy-herbaceous fragrance types, in Gardenia, Jasmin, Rose bases, etc. in trace amounts, or in higher concentration if used as a modifier for Benzyl acetate.

Occasionally used in flavor compositions, mainly in imitation Banana, Raspberry, Strawberry, and in "Tutti-frutti" flavor.

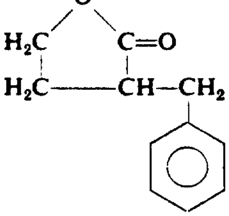
Concentrations are usually about 25 ppm in the finished product.

Prod. from *iso*-Butyric acid and Benzyl alcohol by direct esterification using azeotropic conditions.

G.R.A.S. F.E.M.A. No.2141.

4-22; 5-233; 77-186; 86-24; 103-114; 140-140;

## **295:** alpha-**BENZYL**-gamma-**BUTYROLACTONE**



$C_{11}H_{12}O = 160.22$

Colorless or pale straw-colored, viscous liquid. Sp.Gr. 1.13. B.P. approximately 300° C.

Very faint, sweet-balsamic odor of great tenacity. Sometimes described as resembling the odor of Tolu balsam.

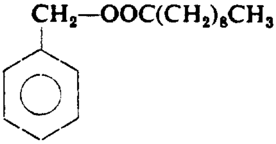
Suggested for use in perfumes as a fixative in heavy floral fragrance types. However, its odor value and odor type are not sufficiently characteristic or unique that this material can stand out alone. It does not offer superior odor value as compared to Tolu balsam, and it is considerably more expensive.

Prod. (several methods), e.g.: from Benzyl malonic ester plus Ethylene oxide.

30-254; 31-170; 86-23; 156-229;

## 296: BENZYL CAPRATE

Benzyl decanoate.
Benzyl decylate.



$C_6H_5CH_2{-}OOC(CH_2)_8CH_3$

$C_{17}H_{26}O_2 = 262.40$

Colorless oily liquid.

Very faint, fatty-waxy, remotely floral odor.

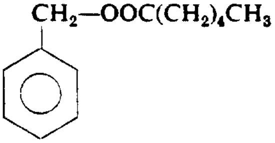
Has been suggested as a fixative in floral compositions, but does not seem to contribute any unique notes.

The author is not aware of its (possible) use in flavors.

Prod. from Benzyl alcohol and Decanoic acid by direct esterification under azeotropic conditions.

## 297: BENZYL CAPROATE

Benzyl hexanoate.
Benzyl hexylate.
Benzyl hexoate.



$C_6H_5CH_2{-}OOC(CH_2)_4CH_3$

$C_{13}H_{18}O_2 = 206.29$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Sweet, mild-fruity, slightly green odor, reminiscent of Apricot, but with a distinctly floral note.

Occasionally used in perfumes for modifying effect in Jasmin, Gardenia, Tuberose, Lily, etc. usually in combination with lower alifatic esters of Benzyl alcohol.

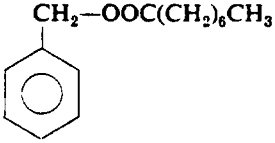
Used in flavor compositions, mainly as a modifier, in imitation Pineapple, Apricot, etc. and in Tutti-frutti flavor.

Prod. by direct esterification of Benzyl alcohol with Hexanoic acid under azeotropic conditions.

86-23; 103-128;

## 298: BENZYL CAPRYLATE

Benzyl octylate.
Benzyl octanoate.
Benzyl octoate.



$C_6H_5CH_2{-}OOC(CH_2)_6CH_3$

$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Flat, but fruity odor, more peachy than Apricot-like, and with a herbaceous-fatty undertone.

Occasionally used in perfumes as a modifier for lower alifatic esters of Benzyl alcohol. In certain floral fragrances, it may be desirable to introduce a fatty-floral note for "petal" effects, and there are cases where Benzyl caprylate can fill such a demand.

Useful in fruity flavor compositions, where the higher boiling ester may act as a fixative for more volatile components. This is important for hard candy, baked goods, etc. where the functional product will be exposed to heat in processing.

Apricot, Peach, Pineapple, etc. Concentrations may not be more than traces.

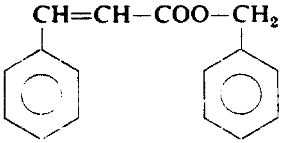
This material is NOT listed in the American G.R.A.S. list.

Prod. by direct esterification of Benzyl alcohol with Octanoic acid under azeotropic conditions.

4-21; 86-23; 103-129;

## 299: BENZYL CINNAMATE

Benzyl-*beta*-phenylacrylate.
"Cinnamein" (this name also used for Benzyl benzoate-plus-Benzyl cinnamate mixture).



$C_{16}H_{14}O_2$ = 238.29

White crystals, granular or powder, melting at 35° C.

Insoluble in water, Propylene glycol and Glycerin. Soluble in alcohol and oils.

Mild, sweet-balsamic and somewhat floral odor of great tenacity.

Used quite frequently in perfumery, mainly as a fixative, and particularly in perfumes for Talcum (powders). It blends well with floral bases, spicy fragrances and Ambre types.

Used in flavor compositions for imitation Apricot, Cherry, Chocolate, Honey, Peach, Pineapple, Liquor, Raspberry, Rum, Prune, etc.

Concentration may be little more than traces, usually about 6 ppm, except in chewing gum: up to 125 ppm.

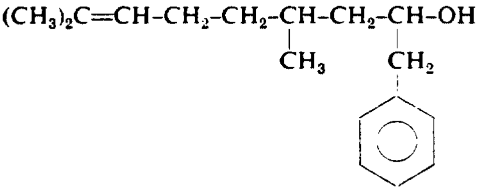
G.R.A.S. F.E.M.A. No.2142.
FCC-1964-797.

Prod.: From Sodium cinnamate and Benzyl chloride (with or without catalyst). Other methods start from Benzyl acetate and Benzaldehyde, using a Claisen type condensation, etc.

4-21; 5-264; 86-23; 100-38; 103-129; 106-72; 156-63; 140-150;

## 300: BENZYL CITRONELLOL

(Presumably): *l*-Benzyl citronellol.



$C_{17}H_{26}O$ = 246.40

Colorless oily liquid.

Rich, sweet-rosy odor, warmer than that of Citronellol.

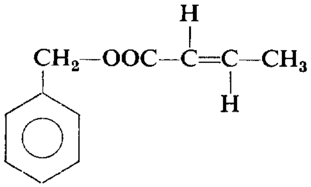
Suggested for use in Rose bases, and generally in floral base.

Very rarely offered commercially.

4-21; see also: (30-406);

## 301: BENZYL CROTONATE

Benzyl-*alpha*-crotonate. (See NOTE below).
*5*-Benzyl-*trans-2*-butenoate.
Benzyl-*beta*-methylacrylate.



$C_{11}H_{12}O_2$ = 176.22

Colorless or very pale straw-colored oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-herbaceous, mildly spicy, but not pungent odor of moderate tenacity.

This ester is one of many esters of unsaturated acids to become of perfumery interest within the past decade or so. The Tiglates and Angelates represent a similar line of esters of interest to the creative perfumer and to the perfumer working on artificial essential oils.

The warm, herbal notes are particularly interesting because they display such versatility that the perfumer soon will find himself using these esters in Rose, Lavender, Ambre, Oriental, Fougere, etc. and in the reconstruction of essential oils, all because these esters lend "natural" notes and warmth to the composition.

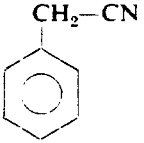
The title ester blends particularly well with "tabac" notes in modern fragrances, with Oakmoss and Styrax, Opopanax, etc. in novel type "Oriental" fragrance, etc.

Prod.: by direct esterification of Crotonic acid with Benzylalcohol under azeotropic conditions.

Note: Commercial Crotonic acid usually contains significant amounts of Allo-crotonic acid, also known as *cis*-Crotonic acid, or *iso*-Crotonic acid.

## 302: BENZYL CYANIDE

Phenyl acetonitrile.



$C_8H_7N = 117.15$

Colorless mobile liquid. B.P. 234° C.
Sp.Gr. 1.02.

Very slightly soluble in water, soluble in alcohol and oils.

Peculiar herbaceous-green, yet very sweet and heavy-floral in its undertones. It is reminiscent of the odor of Orange leaf water absolute, also of Orange flower water absolute.

The recent introduction of Nitriles into perfumery has partly been supported by the fact that many Nitriles have odors closely resembling that of the corresponding Aldehyde, yet the Nitrile is stable in alkali. Benzyl cyanide forms an outstanding exception from the theory of odor similarity between the Nitriles and the Aldehydes. It has little, if anything at all, in common with Phenyl acetaldehyde in odor.

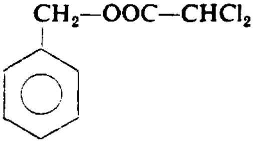
Benzyl cyanide (absolutely pure) is interesting for use in Jasmin, Tuberose, Orange flower substitutes, bases, etc. and in general as a powerful herbaceous-green note in heavy floral fragrances.

As mentioned above, it is stable in alkali, but it will break down in mild acid. It is also likely to react with aldehydes over a sufficiently long period of time.

Prod.: From Benzyl chloride and Sodium cyanide.

68-598; 77-212; 86-23; 90-822; 140-175; 100-138;

## 303: BENZYL DICHLORO ACETATE



$C_9H_8Cl_2O_2 = 219.08$

Colorless viscous oil. Sp.Gr. approximately 1.35.

Mild, but intensely sweet, floral odor in the Jasmin-Orange flower theme. Excellent tenacity.

This ester, when absolutely pure and free from Dichloroacetic acid could be used in perfumes as a modifier-fixative for floral notes of the mentioned type.

However, the hazard of having only a trace of free acid liberated in the perfume is enough to prohibit the general use of this ester. The acid is extremely corrosive, and is actually used in medicine to remove undesirable skin-growth, warts, etc.

Esters of this acid and the Monochloroacetic acid, as well as the Trichloroacetic acid have been prepared and appear to have interesting odors. However, only the Benzyl monochloroacetate has reached more than experimental stage with the perfumers.

Prod. from Dichloro acetic acid and Benzyl alcohol by direct esterification under azeotropic conditions.

## 304: BENZYL DIETHYL-(2:6-XYLYLCARBAMOYL METHYL)-BENZOATE

"Bitrex" THS-839.

This material, which has no use as an active perfume chemical, and is not used as an active ingredient in food flavors, is mentioned because it has been approved by many authorities as a denaturing agent for Ethyl-alcohol in a number of countries, including the U.S.A.

It is a white powder, slightly soluble in water, soluble in alcohol and some oils.

Practically odorless, but the observer will find an extremely powerful effect of bitter taste in the mouth even after very careful "smelling" of this material, or just after opening a container of it.

The taste is intensely bitter, and perceptible at concentrations well below 1 ppm. However, many substances are known with bitter taste perceptible below 1 ppm:

Quinine (hydrochloride) in aqueous solution is perceptible at about 0.5 ppm.

Strychnine at about 0.2 ppm and

Brucine at about 0.005 ppm.

The authorities concerned about alcohol denaturation are, naturally, not seeking a "minimum perceptible" level of bitterness in their selected denaturant, but rather a "maximum-and-hazard-free" level of bitterness. This level is usually much higher than the minimum perceptible.

Accordingly, the title material is used as an approved alcohol denaturant at the level of:

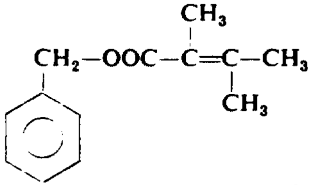
2 grams (or in the U.S.A.: one-sixteenth of one ounce) of the bitter material per 300 kilos (100 U.S. gallons) of alcohol.

In the U.S.A., this is equivalent to 5.8 ppm. The above amount of "Bitrex" replaces 3 ounces of Brucine sulfate, which has been scarce or temporarily unavaiable during the past 10 years. In other words, "Bitrex" is considered 48 times as bitter as Brucine. Although taste perception is extremely subjective, it is safe to say that "Bitrex" is the most bitter substance known. There are people who can detect the bitterness of "Bitrex" at concentrations near 0.001 ppm – or one part in 1000 Million parts of water.

"Bitrex is considered about 250 times as bitter as Glucose octaacetate, a bitter chemical used for alcohol denaturing, and for flavors, see monograph in this work.

## 305: BENZYL-2,3-DIMETHYL CROTONATE

Benzyl methyl tiglate.



$C_{13}H_{16}O_2 = 204.27$

Colorless oily liquid, insoluble in water. Soluble in alcohol and oils.

Warm-herbaceous-ethereal odor with fruity-spicy character, quite powerful.

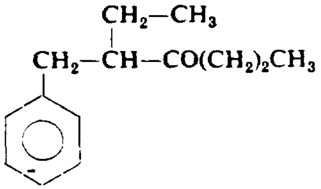
Very rarely offered commercially.

Used in fruit and spice flavor types, usually in traces only.

G.R.A.S. F.E.M.A. No.2143.

## 306: BENZYL DIPROPYLKETONE

(Morellone) (trade name).
*3*-Benzyl-*4*-heptanone.
*1*-Phenyl-*2*-ethyl-*3*-hexanone.



$C_{14}H_{20}O = 204.31$

Colorless oily liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Mild, but rich-fruity, sweet, Plum-like, marmelade-like odor with a peculiar minty-herbaceous character.

Powerful and sweet-Plum-like taste.

Used in fruit flavors, mainly for Cherry (the European, non-Benzaldehydic type), Apricot, Plum, Peach. It blends excellently with Rum flavor materials and introduces quite "natural" character and richness to the imitation flavors.

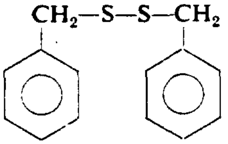
Concentrations are usually as low as 10-12 ppm in the finished product.

This ketone is high-boiling and performs well under conditions where heat is involved (baked goods, hard candy etc.).

G.R.A.S. F.E.M.A. No.2146.

## 307: BENZYL DISULFIDE

Dibenzyl disulfide.



$C_{14}H_{14}S_2 = 246.40$

Pale yellowish leafy crystals. M.P. 74° C.
Decomposes before boiling (270° C.).

Very slightly soluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and in oils.

Powerful "burnt-caramellic" aroma, unpleasant at high concentration but resembling the odor of roasted carbohydrates when sufficiently diluted.

Used in Coffee and Caramel flavors.

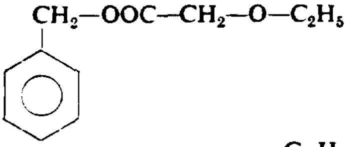
Concentrations are usually about 6-7 ppm. in the finished consumer product.

Prod. (among several methods), e.g.:
1) from Benzyl chloride and $Na_2S_2$.
2) from Benzyl mercaptan by oxidation.

G.R.A.S.

26-428; 90-830; B-IV-465; 68-504;

## 308: BENZYL ETHOXYACETATE



$C_{11}H_{14}O_3 = 194.23$

Colorless liquid.

Sweet floral odor, reminiscent of the odors of Benzyl acetate and Benzyl propionate, sweeter, less pungent than that of the acetate, not as fruity as that of the propionate.

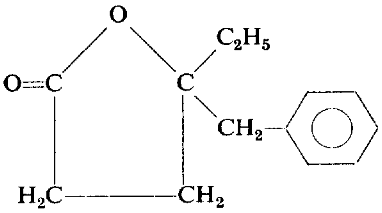
Has been suggested for use in perfumery as a modifier for the named esters of Benzyl alcohol. However, this ester does not offer any significant advantage over those, and the cost of the ethoxyacetate puts it out of competition with the conventional esters.

Prod. by direct esterification of Ethoxyacetic acid with Benzylalcohol.

3-214; 30-288; 159-462;

## 309: BENZYL ETHYL BUTYROLACTONE

Ethyl benzyl-*gamma*-butyrolactone.



$C_{13}H_{16}O_2 = 204.27$

Colorless or pale straw-colored oily liquid. Almost insoluble in water, soluble in alcohol, miscible with oils.

Sweet balsamic and very tenacious odor.

This lactone represents a group of comparatively rare and not very interesting derivatives of Butyrolactone. In search of useful materials for perfumes and flavors, this was developed among scores of other, equally unsuccessful, alkyl-*gamma*-lactones.

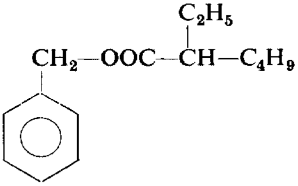
If the material were made available and marketed at a reasonable cost, it could possibly find use as a fixative in heavy floral fragrance types, including those where Ylang-Ylang is employed.

In the author's opinion, there is no true need for this material in perfumes or flavors.

Prod.: (several methods) e.g.: from Benzyl ethyl ethylene oxide with Sodio-malonic ester.

## 310: BENZYL ETHYLCAPROATE

Benzyl-2-ethylhexanoate.
Benzyl ethylhexylate.
Ethyl butyl acetic acid, Benzylester.



$C_{15}H_{22}O_2 = 234.34$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, oily-herbaceous, almost earthy odor with only a trace of fruity notes. Good tenacity.

The taste shows more pronounced fruity notes in concentrations below 20 ppm. Higher concentrations seem herbaceous or fungal, mushroomy.

This ester has been suggested for use in perfumes and flavors, but it is not regularly offered from the normal sources of such chemicals. It is rarely offered under its proper chemical name, in fact.

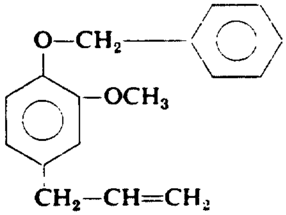
Although the acid from which it is derived is a very common derivative from petrochemical research (*iso*-Butane derivative), there seems to be little chance that the ester will become a popular fragrance or flavor chemical.

Prod.: from Benzyl alcohol and Ethyl butyl acetic acid.

## 311: BENZYL EUGENOL

Eugenol benzylether.

Note: Do not confuse this ether with Benzoyl eugenol which is Eugenol benzoate. (See Benzoyl eugenol).



$C_{17}H_{18}O_2 = 254.33$

Colorless prismatic crystals. M.P. 30° C.

Very faint, warm-spicy odor with a haylike undertone. Like most other crystalline materials, it can display a range of unusual odors mostly deriving from surface adsorption.

The odor of the material itself is best evaluated when dissolved in an odorless solvent, e.g. Diethyl phthalate. A 5% solution in this solvent has hardly any odor at all.

Insoluble in water, poorly soluble in Propylene glycol, somewhat soluble in alcohol, soluble in oils.

Mainly used as a fixative in heavy floral fragrance types, in Carnation and many types of spicy fragrances, and as a sweetener along with Rose fragrances, etc.

It seems to be much less popular than the Benzyl-*iso*-eugenol (see next monograph). The latter being sweeter and more versatile in use.

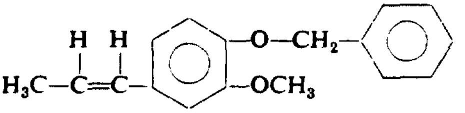
Prod. from Benzyl chloride and Eugenol in alcoholic Potassium hydroxide (e.g. first step in making the isomer).

4-22; 4-50; 5-280;

## 312: cis-**BENZYL**-iso-**EUGENOL**

*iso*-Eugenol benzylether.

This is the minor component of the commercial product called Benzyl-*iso*-eugenol. It is probably the more desirable component from an odor point of view).



$C_{17}H_{18}O_2 = 254.33$

White or off-white crystalline powder.

M.P. 34° C.

Soluble in alcohol and oils, insoluble in water.

Faintly rosy-balsamic-Carnation type odor of exceptional tenacity. It is overall sweet and generally floral when blended with lower boiling components.

It blends excellently with the Ionones and Benzyl salicylate in Violet bases, and is widely used as a fixative.

This ether is also used in flavor compositions, mainly in Spice flavors, but because of its peculiar "dry" sweetness, also useful in Banana flavors.

Concentrations are usually about 15-16 ppm in the finished product.

G.R.A.S. (The Federal Register does not specify: *cis*- or *trans*-).

Prod. from Benzyl eugenol by isomerization (alcoholic Potass. hydroxide).

4-22; 95-122; 106-76;

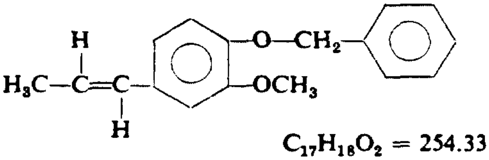
## 313: trans-**BENZYL**-iso-**EUGENOL**

*iso*-Eugenol benzylether.

Benzyl-*2*-methoxy-*4*-propenyl phenyl ether.

*3*-Methoxy-*4*-benzyloxypropenyl benzene.

This is the *major* component of the commercial product called Benzyl *iso*-eugenol. It is probably less desirable from an odor point of view, it is less delicate in odor.



$C_{17}H_{18}O_2 = 254.33$

White or off-white crystalline powder. Soluble in alcohol and oils, insoluble in water. M.P. 57° C.

Very mild floral-spicy odor, balsamic-sweet, delicate. Only in actual use it is reminiscent of certain flowers, such as Carnation, Rose, Magnolia, etc.

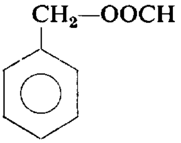
It is an excellent fixative for floral compositions, blends well with Ylang-Ylang, Benzyl salicylate, Rose alcohols, Butyl phenylacetate, etc.

Its use in flavors is described in the previous monograph. The two isomers are not offered commercially as pure *cis*- or pure *trans*-Benzyl *iso*-eugenol.

NOTE: See also notes under *iso*-Eugenol.

Prod. and Literature: see previous monograph.

## 314: BENZYL FORMATE



$C_8H_8O_2 = 136.15$

Colorless liquid. Very slightly soluble in water. Sp.Gr. 1.08. B.P. 202° C. Solidifies in the cold, melts at 4° C.

Powerful, fruity-green, herbaceous-earthy, yet somewhat floral, heavy, but not very tenacious odor.

This ester is one of the chief components in the absolute of the Japanese hedgerose (Hamanasu).

Its odor is amazingly different from that of the Acetate (typical of most -formates).

Very sweet taste, more fruity than floral, spicy Banana-type.

Used quite frequently in perfume compositions, for floral bases such as Jasmin, Gardenia, Neroli, Hyacinth, Carnation, and also in Fougères.

Used in flavor compositions for imitation Apricot, Banana, Cherry, Chocolate, Honey, Liquor, Nut, Peach, Plum, Prune, Pineapple, etc.

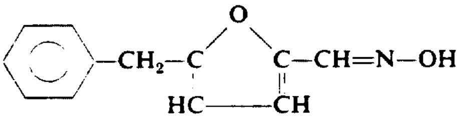
Concentrations are usually about 12-15 ppm in the finished product. In chewing gum the concentration may be as high as 35 ppm.

G.R.A.S. F.E.M.A. No.2145.

Prod. from Benzyl alcohol and Formic acid with a water-removing additive.

4-22; 5-259; 26-430; 77-180; 90-327; 103-84; 106-73; B-VI-435; 156-59; 140-133;

## 315: syn-5-BENZYL-2-FURFURALDOXIME



$C_{12}H_{11}NO_2 = 201.23$

White crystalline powder. Poorly soluble in cold water, slightly soluble in hot water, soluble in alcohol, insoluble in oils, except in certain alifatic esters, etc.

Virtually odorless when pure.

Aqueous solutions of 50-100 ppm have a distinctly sweet taste which is accompanied by a slightly bitter aftertaste similar to that observed with Saccharin.

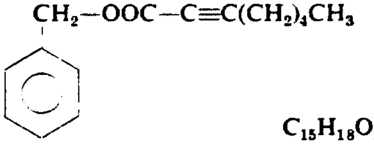
The title material is about 700 times sweeter than cane sugar at normal use concentrations. It is equivalent to 1½ times Saccharin in sweetening power.

The subject material is not generally approved for use as a food sweetener, but it has some academic interest in the study of sweetness of isomers. The *anti*-Aldoxime has only a weak and not expressly sweet taste.

30-146; 159-265; 159-533;

## 316: BENZYL HEPTINCARBONATE

Benzyl octynoate.



$C_{15}H_{18}O_2 = 230.31$

Colorless oily liquid, insoluble in water, soluble in alcohol and oils. B.P. 255° C. Sp.Gr. 1.01.

Oily-green foliage odor with faintly floral undertone.

By some perfumers considered one of the most attractive of all the Acetylenic acid esters (or equal to Amyl heptin carbonate)

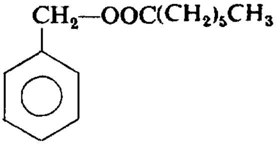
Used as a fixative for Violet topnotes, and occasionally for "special" green effects.

Prod. from *n*-Heptyne sodium and Benzyl chlorocarbonate.

4-22; 86-23; 103-295;

## 317: BENZYL HEPTOATE

Benzyl heptylate.
Benzyl heptanoate.



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils. B.P. 257° C.
Sp.Gr. 0.98.

Herbaceous-fruity odor, remotely reminiscent of the fruity notes in Clary Sage or certain types of Lavender.

Occasionally used in perfumery as a modifier in herbaceous fragrance types (Fougères, etc.) or in novelty types. It may emphasize the freshness of Bergamot, Clary Sage or Lavender when used in such combination.

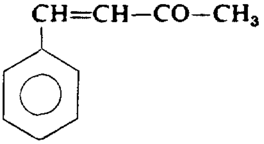
Finds some use in flavor compositions, mainly for Apricot and Peach imitations.

Prod. from Benzyl alcohol and Heptanoic acid by direct esterification under azeotropic conditions.

4-22; 30-286; 86-23; 103-128;

## 318: BENZYLIDENE ACETONE

Methyl cinnamyl ketone.
Methyl styryl ketone.
Benzal acetone.
"Benzylidene ketone" (confusing name).
*4*-Phenyl-*3*-buten-*2*-one.
Cumaranol.
Exists in *cis*- and *trans*-form. (Commercial product is *cis*-isomer).
NOTE: Do not confuse with *Benzyl* acetone.



$C_{10}H_{10}O = 146.19$

Yellowish plate crystals. M.P. 42° C. (*cis*-isomer). M.P. 4° C. (*trans*-isomer).
Sp.Gr. 1.04. B.P. 262° C. Insoluble in water, soluble in alcohol and oils. Also soluble in sulfuric acid solution.

Sweet, but rather pungent odor with a creamy-floral note.

Occasionally used in perfumery for Sweet Pea (used to be a "must" in this type of fragrance), in Appleblossom, etc., often in combination with Neroli and Hyacinth bases.

Also used in flavors, particularly in Chocolate, Cocoa, Cherry, Fruit, Nut, Vanilla, etc. – but usually at very low concentration. Concentration in finished product will rarely exceed 0.2 to 0.5 ppm.

Prod. by Claisen condensation of Benzaldehyde and Acetone.

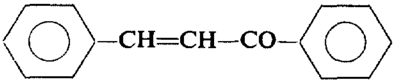
G.R.A.S. F.E.M.A. No.2881.

NOTE: This ketone is repeatedly reported in trade literature as being strongly skin-irritating. It may be that its acceptance in food is approved only because of very low use-concentration.

4-19; 4-22; 5-165; 26-418; 30-179; 31-84; 95-170; 96-150; 100-139; B-VII-364;

## 319: BENZYLIDENE ACETOPHENONE

Benzal acetophenone.
Phenyl cinnamyl ketone.
Chalkone.
Phenyl styryl ketone.
*1*,*3*-Diphenyl-*2*-propen-*1*-one.
Exists in *cis*- and *trans*-forms. (Commercial product is *trans*-isomer).



$C_{15}H_{12}O = 208.26$

Yellowish crystals. M.P. 58° C. (*trans*-isomer). M.P. 46° C. (*cis*-isomer).

Sp.Gr. 1.07 (liquid). B.P. approximately 346° C. Insoluble in water, soluble in alcohol (poorly) and oils.

Sweet floral, balsamic and heavy odor, somewhat herbaceous-warm undertone.

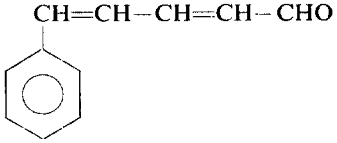
Is occasionally mentioned in perfumery literature, but the author of this work believes that the use of Benzylidene acetophenone is very limited if not completely abandoned.

Prod. by condensation of Benzaldehyde with Acetophenone.

68-1183; 103-271; 100-228;

## 320: BENZYLIDENE CROTONALDEHYDE

*5*-Phenyl-*2*,*4*-pentadienal.
Cinnamylidene acetaldehyde.



$C_{11}H_{10}O = 158.20$

Yellowish oily liquid.

Oily-spicy, warm, balsamic and very tenacious odor. The commercial product is a by-product and often used in the crude state, dark of color, resinous of odor.

This aldehyde finds some use in perfume compositions, mainly in industrial fragrances where its low cost is an advantage and its color (and tendency to discolor) are of no great disadvantage.

It blends well with Peru balsam, Tolu balsam, Copaiba, Amyl salicylate, Ocotea oil or Chinese Camphor oil fractions, etc. in various compositions for masking, etc.

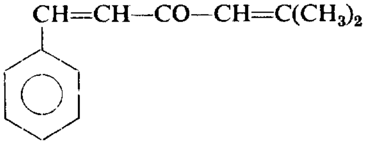
Prod.: The aldehyde occurs as a result of "double addition" of Acetaldehyde to Benzaldehyde in the process of making Cinnamic aldehyde. The Acetaldehyde may continue to add to the Cinnamic aldehyde under certain (improper) conditions, and the Acetaldehyde may also form polymers of its own by self-condensation.

The title aldehyde is higher boiling than Cinnamic aldehyde and the separation of the two presents no technical problem.

3-266; 86-23;

## 321: BENZYLIDENE MESITYLOXIDE

Benzal mesityloxide.
Cinnamyl-*iso*-butylidene ketone.
*1*-Phenyl-*5*-methyl-*1*,*4*-heptadien-*3*-one.



$C_{13}H_{14}O = 186.26$

Colorless liquid.

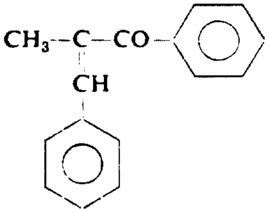
Rather sharp, fruity odor, somewhat reminiscent of Strawberry.

Recommended for use in flavor compositions, but is NOT included in the G.R.A.S. list issued by the Federal Register, U.S.A.

Prod. from Benzaldehyde by Claisen condensation with Mesityloxide (*4*-Methyl-*3*-penten-*2*-one).

31-84;

## 322: alpha-BENZYLIDENE PROPIOPHENONE



$C_{16}H_{14}O = 222.27$

Viscous yellowish oil, solidifying in the cold. B.P. approximately 310° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-creamy, floral-balsamic tenacious odor. In dilution quite floral in the Sweet-Pea type, at higher concentrations it shows tendency of supplying spicy-warm notes.

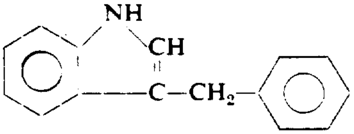
This ketone, rarely offered under its proper chemical name, is used in perfumery, mainly in specialties and floral-balsamic bases, in Fougere or Lavender additives, etc. It is quite powerful and has natural-lifting effect upon floral as well as non-floral fragrance types. Use concentration will normally be about 0.5 to 1.5 % in a finished perfume oil.

Prod.: by condensation of Benzaldehyde with Propiophenone.

86-23;

## 323: beta-BENZYL INDOLE

*3*-Benzylindole.



$C_{15}H_{13}N = 207.28$

White crystals. M.P. 103° C. Almost insoluble in water, soluble in alcohol and oils.

Floral-earthy, slightly mushroom-like odor (Champignon-like).

By some perfumers considered one of the most attractive and interesting derivatives of Indole. When absolutely pure, it has no trace of Skatole-type notes, and it offers an entirely different type of floralness if used as a modifier of Indole.

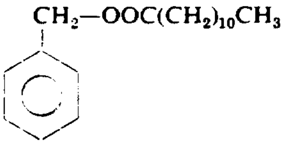
Very rarely offered commercially under its proper chemical name.

Prod. from Indole by reaction with Sodium in Benzylalcohol.

5-313; 69-84; 86-24;

## 324: BENZYL LAURATE

Benzyl dodecylate.
Benzyl dodecanoate.



$C_{19}H_{30}O_2 = 290.45$

Colorless oily liquid. Sp.Gr. 0.94.

Very faint, fatty odor. Probably odorless to most people when this ester is absolutely pure.

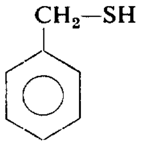
Has been suggested as carrier solvent for alifatic aldehydes in perfume compositions. Occasionally it may form part of the desirable, fatty notes in Jasmin, Gardenia, Neroli, etc.

Prod. from Benzyl alcohol and Lauric acid (Dodecanoic acid) by direct esterification under azeotropic conditions.

4-22; (incorrect info.); 86-24; 106-78;

## 325: BENZYL MERCAPTAN

*alpha*-Toluene thiol.
Benzyl thiol.



$C_7H_8S = 124.21$

Colorless or pale straw-colored mobile liquid. Practically insoluble in water, soluble in oils. B.P. 194° C.

The odor is most frequently described as "Leek-like", which – in the author's opinion – is a more exact description than the older, still common "onion-like". It has the sharpness of Leek odor, yet not lachrymatory.

This sulfur compound has been suggested for use – and is actually used – in Coffee imitation flavor. Concentration is usually mere traces.

It is interesting to note, that publications, such as the comprehensive and recent, very highly regarded, (Litt. 158-442, Dr. Gianturco) do NOT include this mercaptan in their findings in analysis of roasted Coffee. Many lower mercaptans are known components of roasted Coffee. In fact, very few *Benzyl* derivatives are present in natural food products.

Benzyl mercaptan is a comparatively unstable chemical. It reacts with Aldehydes, Ketones, etc. and it may oxidize to Benzyl disulfide or further to Benzaldehyde – Benzoic acid.

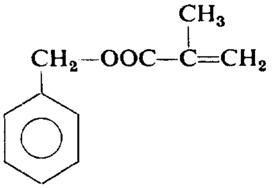
Prod. from Benzyl chloride plus Potassium hydrosulfide.

G.R.A.S. F.E.M.A. No.2147.

68-503;

## 326: BENZYL METHACRYLATE

Benzyl-*alpha*-methylacrylate.
Benzyl propen-*1*-carboxylate.



$C_{11}H_{12}O_2 = 176.22$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Soft, warm, herbaceous-rosy odor of moderate tenacity.

This ester has found some use in perfume compositions where it may introduce very desirable notes in Rose and other floral fragrances, in Chypre, Oriental and heavy woody fragrance types, etc.

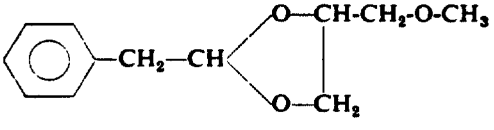
It blends excellently with Oakmoss, Vetiver, Phenylacetaldehyde dimethylacetal, Citronellol, as well as with Lavender, Lavandin, Spike Lavender, etc. The ester is also used in soap and detergent perfumes, where its low cost allows for a more liberal application.

See also Phenyl ethyl methacrylate.

Prod.: from Phenylethyl alcohol and Methacrylic acid. Also directly from Acetone cyanhydrin when Benzyl alcohol is present in the reaction.

## 327: 2-BENZYL-4-METHOXYMETHYL-1,3-DIOXOLAN

Phenylacetaldehyde methoxypropyleneglycol acetal.



$C_{12}H_{16}O_3 = 208.26$

Colorless, slightly voscous liquid.
B.P. 260° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral and tenacious Hyacinth-green odor.

This acetal could, according to the description, seem to be "just another Hyacinth acetal", and we do have plenty of them in perfumery. But it has a very pleasant "juicy-fresh" greenness about its odor, a note which seems to be more or less inherent in many ether-acetals.

The material is rarely offered under its proper chemical name, but it is not difficult to prepare, and it is made from inexpensive raw materials.

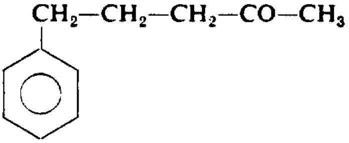
Prod.: from Glycerol-*1*-methylether plus Phenylacetaldehyde by condensation. (See NOTE).

5-323; 86-24; 155-187;

NOTE: Glycerol-*2*-methylether is also known, but less likely to be used, since it is much more difficult to prepare.

## 328: BENZYL METHYL ACETONE

(The title name is somewhat confusing).
Methyl hydrocinnamyl ketone.
Methyl phenylpropyl ketone.
*5*-Phenyl-*2*-pentanone.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid. Very slightly soluble in water, soluble in alcohol and oils.

Sweet, fruity-floral, slightly balsamic odor of moderate tenacity.

This ketone, mostly sold under various trade names, has found very little use in perfumes. Many newer, related materials have been much more successful, particularly those containing a hydroxyl- or a methoxy-radicle in the ring, preferably in the *para*-position.

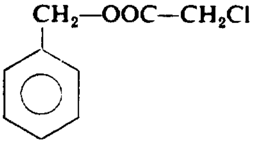
The subject ketone blends very well with members of the Cinnamic family, with Salicylates and Coumarin. It lends sweetness to floral fragrances, sweet-woody notes in Mimosa or Cassie bases, and it rounds off the harshness of overly fruity topnotes. It also seems to improve the effect of Ethyl methyl phenyl glycidate as a fruity item.

The author is not aware of this material being used in flavors.

Prod.: by reduction of Phenyl ethylidene acetone, which is obtained from Phenylacetaldehyde by condensation with Acetone.

## 329: BENZYL MONOCHLORO ACETATE

Benzyl chloracetate.



$C_9H_9ClO_2 = 184.63$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.22.

Mild, Jasmin-type odor, floral-fruity, of considerable tenacity.

Could find use in Jasmin, Lilac, Appleblossom fragrances, particularly for soap, where this ester has greater fixative effect than the Benzyl acetate.

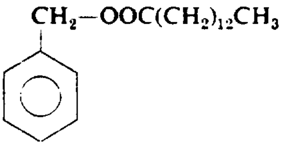
However, this ester must be absolutely acid-free to be permitted or recommended for use in any cosmetic product. The acid is highly corrosive. Older odor-descriptions of this ester seem to indicate that the product has not always been very pure.

Prod. from Benzyl alcohol and Monochloroacetic acid by direct esterification under azeotropic conditions.

4-22; 5-265; 86-24; (and private experiments).

## 330: BENZYL MYRISTATE

Benzyl tetradecanoate.



$C_{21}H_{34}O_2 = 318.50$

Colorless, oily liquid.

The comments given under *Benzyl laurate* also pertain to this ester.

It has been suggested for use as a solvent/fixative/blender, a diluent for alifatic aldehydes, a blender for Orris fragrances or bases.

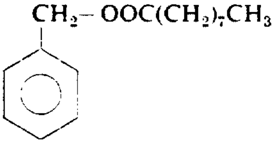
Overall, it has little interest to the perfumer.

Prod. from Benzyl alcohol and Myristic acid by direct esterification under azeotropic conditions.

4-22;

## 331: BENZYL PELARGONATE

Benzyl nonanoate.
Benzyl nonylate.



$C_{16}H_{24}O_2 = 248.37$

Colorless liquid. Sp.Gr. 0.962.

Faint, but fresh-balsamic, slightly fatty odor.

Although mainly suitable as a solvent of low odor level, this ester could be used as a blender/modifier in Oriental fragrance types, in Citrus fragrances (where it could act partly as a fixative) and in Fougeres, etc.

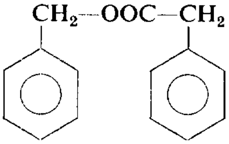
However, it does not seem to have gained much popularity among creative perfumers.

Prod. from Benzyl alcohol and Nonoic acid by direct esterification under azeotropic conditions.

4-22; 86-24; 103-129;

## 332: BENZYL PHENYLACETATE

Benzyl-*alpha*-toluate.



$C_{15}H_{14}O_2 = 226.28$

Colorless, slightly viscous liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils. B.P. 317° C. Sp.Gr. 1.10.

Mild, sweet, honey-floral odor, the honey note being almost imperceptible in pure material. In fact, a pure ester has an extremely faint odor.

Used in perfumes for floral fragrances, Oriental bases, etc. It has an exceptionally good tenacity, and is very stable in soap, where its fixative effect is frequently utilized.

Used quite commonly in flavor formulations, for imitation Butter, Caramel, Fruit, Honey, etc. Again here, its fixative effect makes it suitable for flavors for hard candy, baked goods, etc., since this ester has good heat-stability.

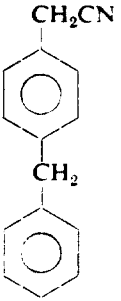
G.R.A.S. F.E.M.A. No.2149.

Prod. by direct esterification of Benzyl alcohol with Phenylacetic acid under azeotropic conditions.

4-22; 5-271; 86-24; 103-129; 106-79; 155-90;

## 333: para-BENZYL PHENYLACETONITRILE

*para*-Benzyl benzylcyanide.



$C_{15}H_{13}N = 207.28$

Colorless viscous liquid. B.P. higher than 300° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Peculiar warm, nutlike and fruity, deep-sweet and oily odor of excellent tenacity.

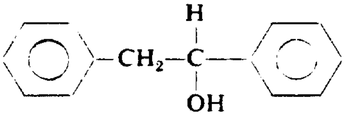
This rare material has been suggested for use in perfume compositions as a modifier/blender in heavy floral fragrances, e. g. Gardenia, Tuberose, etc. – also as a companion to Nonalactone. Some observers find a similarity to Nonalactone in the title material.

It is rarely, if ever, offered under its proper chemical name, but it may be prepared by the individual users.

163-181;

## 334: BENZYL PHENYL CARBINOL

Phenyl benzyl carbinol.



$C_{14}H_{14}O = 198.17$

White crystalline powder. M.P. 65° C.

Mild floral, somewhat Orris-like odor.

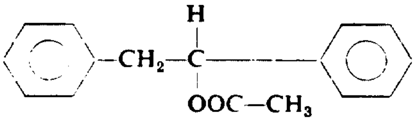
This is one of a series of "carbinols" manufactured several decades ago by one European perfume chemical manufacturer. Only a few out of dozens marketed (and hundreds known) of these "carbinols" and their esters have ever become standard items on the perfumers' shelves. This simple carbinol does not seem to have interesting notes to such a degree that it will survive the competition with the hundreds of other perfume chemicals annually marketed.

Prod. from (several methods), e. g. Styrene oxide and Phenyl magnesium bromide.

44-162; 103-291; 156-76;

## 335: BENZYL PHENYL CARBINYL ACETATE

Phenyl benzyl carbinyl acetate.



$C_{16}H_{16}O_2 = 240.30$

Colorless, slightly viscous liquid.

Fresh-floral, somewhat green odor, rather dry (compared to Dimethyl Benzyl carbinyl acetate), and not as versatile, on account of the lack of sweetness.

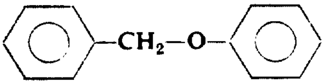
See notes under Benzyl phenyl carbinol.

Probably of very little interest to the creative perfumer.

Prod. by direct esterification of Benzyl phenyl carbinol.

## 336: BENZYL PHENYL ETHER

Phenyl benzyl ether.
Benzyl phenyl oxide.



$C_{13}H_{12}O = 184.24$

White crystalline mass. M.P. 39° C.
B.P. 286° C.

Faint, sweet and remotely floral odor. However, most commercial products seem to have a pronounced "Bitter Almond" note, probably deriving from impurities in this chemical.

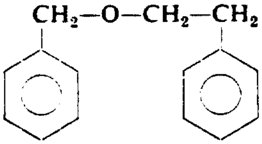
Besides, this ether does not seem to offer any unusual or specifically desirable notes which are not obtainable by means of other and equally inexpensive perfume chemicals.

Prod. from Benzyl chloride and Sodium phenolate solution.

68-502; 86-114; 163-232; 163-371;

## 337: BENZYL PHENYLETHYL ETHER

Phenylethyl benzyl ether.



$C_{15}H_{16}O = 212.29$

Colorless oily liquid.

Heavy floral-earthy-mossy, "wet-green" odor, reminiscent of certain types of Rose. However, this ether is only pleasant smelling when properly diluted.

This chemical forms member of a long series of ethers offered on the market partly as a result of intense research concentrating on the identification of components in powerfully smelling natural flower oils.

The East Indian (originally Polynesian) Pandanus has very fragrant flowers (see S. Arctander: Perfume and Flavor Materials of Natural Origin, 1960, page 502/504) and the chief component of the flower oil is Methyl-*beta*-phenylethyl ether.

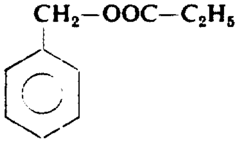
Later chemical research developed a series of ethers, not only the Ethyl phenylethyl ether, but also the Benzyl-, and later even the Phenylethyl ethers of alkoxy-substituted Benzyl alcohol. Among these latter are found some of the most powerfully smelling Rose-chemicals, widely used in successful Rose bases.

Benzyl phenylethyl ether is very stable in soap, and could find use as a modifier for other Rose-fixatives for soap perfumes.

Prod. from Benzyl alcohol and Phenylethyl alcohol, by ether-condensation.

## 338: BENZYL PROPIONATE

Benzyl propanoate.



$C_{10}H_{12}O_2 = 164.20$

Colorless liquid. B.P. 222° C. Sp.Gr. 1.03.

Practically insoluble in water, insoluble in Glycerin, poorly soluble in Propylene glycol and Mineral oil, soluble in alcohol and oils.

Fruity-sweet odor with pronounced floral undertone, overall type Jasmin. Less sharp, and more fruity than the acetate.

Widely used as a modifier for Benzylacetate in Jasmin and – to a lesser degree – in Rose fragrances. Also generally as a floral-fruity, fresh note in floral and Oriental fragrances.

Used in flavor compositions for imitation Apple, Banana, Berry, Grape, Pear, Pineapple, etc.

Concentrations in finished product will usually be about 40 ppm. In chewing gum it may be as high as 150 ppm.

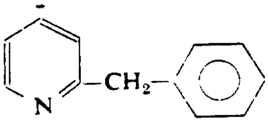
G.R.A.S. F.E.M.A. No.2150.
FCC-1964-799.

Prod. by direct esterification of Benzyl alcohol with Propionic acid (or Propionic anhydride).

4-22; 68-503; 106-80; 156-59; 156-64; 103-106;

## 339: 2-BENZYL PYRIDINE

*alpha*-Benzyl pyridine.



$C_{12}H_{11}N = 169.23$

Pale straw-colored oily liquid. Poorly soluble in water, soluble in alcohol and oils.

Powerful green vegetable type odor with considerable resemblance to the odor of raw stringbeans (or "Haricots-verts"). The warm-herbaceous undertone is often accompanied by traces of a protein-like terminal note, possibly impurity-odor. Moderate tenacity.

This material is included in the present work as an example of the many highly interesting odorous chemicals belonging to a group of organic chemicals normally not considered for fragrance chemical research. Literature has brought scattered reports on alkyl-substituted Pyridines, and the use of Piperidine, Methyl nicotinate and other Amines is known, but not frequently discussed.

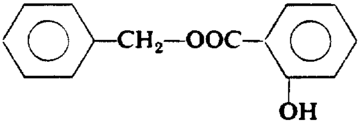
Since the use of several related materials is approved for food flavors, there is reason to assume that a restricted use of Pyridine derivatives could be recognized as well, at least in perfumes.

The subject material could be quite interesting as a novel note in the very fashionable "green" theme in modern fragrances. It might also serve as a trace component in the reconstruction of essential oils and flower absolutes, etc.

(Sample: Reilly Tar & Chemical Co., Inc. U.S.A.).

## 340: BENZYL SALICYLATE

Benzyl-*ortho*-hydroxybenzoate.



$C_{14}H_{12}O_3 = 228.25$

Colorless oily liquid, or opaque crystalline mass, melting at 24-26° C. It may remain supercooled for a considerable length of time. Sp.Gr. 1.18. B.P. 300° C.

Almost insoluble in water, insoluble in Glycerin, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Very faint, sweet-floral, slightly balsamic odor. This ester is, according to the judgment of some people (including perfumers) absolutely odorless, while others find it "musky" of odor. Trace impurities can greatly influence the odor of this high-boiling chemical.

Widely used as a blender in perfumery, and generally as a mild, floral background with an effect not unlike that of Ylang-Ylang (except for power and topnote). Excellent in all florals, Carnation, Wallflower in particular.

Frequently used in flavor compositions. Characteristic of this mild-smelling material is that it has quite powerful taste (insolubility in water may be one of the reasons). It is used in mere traces in Apricot, Banana, Peach and Plum, as well as in the so-called "floral" flavors, where the sweet taste of Benzyl salicylate gives powerful effect.

Prod.

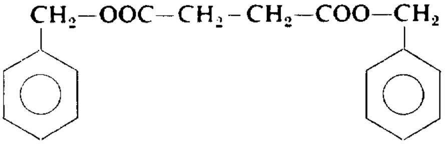
1) from Benzyl chloride and Sodium salicylate (sometimes with an Amine as a catalyst).
2) by Trans-esterification of Benzyl alcohol with Methyl salicylate with Sodium Methyl salicylate catalyst.

G.R.A.S. F.E.M.A. No.2151.
FCC 1964-801.

4-23; 5-264; 77-193; 86-24; 90-574; 95-188; 106-81; 156-62; 103-129; 26-430; B-X-80; 85-156; 140-150;

## 341: BENZYL SUCCINATE

Dibenzyl succinate.
"Spasmin".
NOTE: Mono-Benzyl succinate is known (M.P. 59° C.).



$C_{18}H_{18}O_4 = 298.34$

Leafy crystals or crystalline powder.
M.P. 46° C. B.P. approximately 340° C. (decompos.).

Insoluble in water, soluble in alcohol and oils.

Practically odorless when pure.

Has been suggested as a solvent/blender/fixative in perfume compositions. However, it does not seem to offer very substantial advantages over Diethyl phthalate or other odorless solvents, available at very low cost.

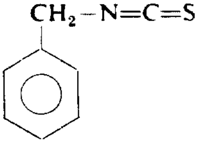
It is true, that this ester, like D.E.P., will influence the odor of a perfume composition in which it is incorporated at a level of more than a few percent. The low vapor pressure of this ester can be changed when it is combined with other odorants of higher vapor pressure.

Prod. by direct esterification of Benzyl alcohol with Succinic acid under azeotropic conditions.

4-43; 26-480; 100-142; B-VI-436; 68-503;

## 342: BENZYL-iso-THIOCYANATE

"Benzyl mustard oil".



$C_8H_7NS = 149.22$

Pale yellowish or almost colorless oil.
Sp.Gr. 1.13. B.P. 243° C.

Insoluble in water, soluble in alcohol and oils.

Very powerful Cress-odor, Watercress type, green-herbaceous, pungent.

Although a chief component of a natural plant, used in foods, this chemical is NOT included in the G.R.A.S. list of the American Federal Register. It is one of comparatively few natural Benzylderivatives, and there is only a small number of Benzyl derivatives included in the G.R.A.S. list.

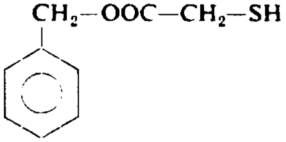
The material is included in this work because it undoubtedly finds use in flavor compositions in a number of countries, mainly in making artificial condiment flavorings, seasonings, etc.

Prod. (synth.)
1) from Benzylamine via Thiuramdisulfide via Sodiumsalt with Iodine to Benzyl-*iso*-thiocyanate.
2) from Benzylamine and Thiocarbonyl chloride.

12-98; 26-430; 30-423; 65-740; 68-492; 90-845; 95-208; 96-234; B-XII-1059; 140-177;

## 343: BENZYL THIOGLYCOLATE

Benzyl mercaptoacetate.



$C_9H_{10}SO_2 = 182.25$

Colorless viscous liquid. Sp.Gr. 1.165.

See comments listed under the monograph: Amyl thioglycolate.

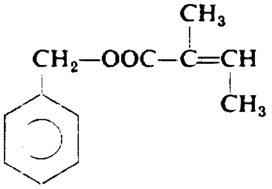
Probably of no interest to the creative perfumer. The odor of this ester is very faint and uncharacteristic.

Prod. from Benzyl alcohol and Thioglycollic acid.

34-1245;

## 344: BENZYL TIGLATE

Benzyl-*trans-alpha*-methylcrotonate.
Benzyl-*trans-alpha-beta*-dimethylacrylate.



$C_{12}H_{14}O_2 = 190.24$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Peculiar fungus-like, mushroom-type odor with a rosy undertone.

Has been suggested for use in Rose fragrances, where this particularly deep-earthy, almost musty undertone can be desirable, e.g. in combination with spicy undertones. This ester also introduces a certain naturalness of herbaceous character, and blends well with Vetiver oil, Oakmoss, etc. in Reseda and similar fragrance types.

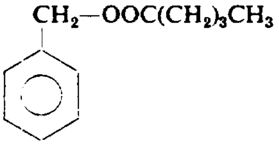
Suggested for use in Rose type fragrances, mainly as a background note and fixative.

Prod. by direct esterification of Benzyl alcohol with Tiglic acid under azeotropic conditions.

4-23; 77-188;
see also footnote under: *iso*-Amyl tiglate.

## 345: BENZYL VALERATE

Benzyl-*n*-pentanoate.
Benzyl valerianate.
NOTE: Commercial product is usually: Benzyl-*iso*-valerate (see next monograph).



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils. B.P. 250° C.

Powerful fruity and somewhat musky, animal-like odor. The odor is less floral and more musky than that of the *iso*-valerate.

Occasionally used in perfumes. It can introduce quite interesting notes in Rose fragrances and in Oriental type fragrances, where the effect can be directed towards the more warm-herbaceous, tobaccolike character.

The *n*-valerate is sometimes preferred for Tobacco flavoring, while the *iso*-valerate is generally preferred for Apple flavor compositions.

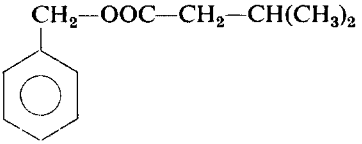
Prod. by direct esterification of Benzyl alcohol with *n*-Valeric acid under azeotropic conditions.

NOTE: The American Federal Register specifies the *iso*-Valerate on the G.R.A.S. list.

4-25; 5-239; 5-263; 140-141;

## 346: BENZYL-iso-VALERATE

Benzyl-*iso*-pentanoate.
Benzyl-*3*-methylbutyrate.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Sp.Gr. 0.99. B.P.246° C.

Insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils.

Powerful, fruity-herbaceous odor with a slightly musky undertone, reminiscent of cured tobacco leaves.

Sometimes used in perfume formulations for Oriental fragrance types – blends well with Opopanax – in Rose bases, Fougeres, and in novelty type fragrances (Tobacco-effect, etc.).

It is somewhat fresher-floral than the *n*-valerate.

Used in flavor compositions for imitation Apple, Apricot, Banana, Cherry, Cheese, Pineapple, Raspberry, Walnut, etc.

It is also suggested for use in Tobacco flavors.

Concentrations are usually about 50 ppm in the finished product, but may be as high as 200 ppm in chewing gum.

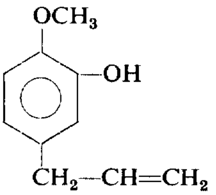
G.R.A.S. F.E.M.A. No.2152.

Prod. by direct esterification of Benzyl alcohol with *iso*-Valeric acid under azeotropic conditions.

3-21; 4-23; 5-239; 5-262; 77-186; 103-123; 106-77;

## 347: BETELPHENOL

Chavibetol.
*2*-Methoxy-*5*-allyl phenol.
*1*-Methoxy-*2*-hydroxy-*4*-allylbenzol.
*5*-Allyl guaiacol.



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid. Solidifies in the cold, melts at 9° C. Sp.Gr. 1.07. B.P. 255° C.

Powerful, sweet-medicinal-spicy odor, reminiscent of tanned leather, smoke and dry wood. In dilution reminiscent of the smokey-dry odor of Chinese tea.

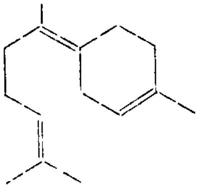
Could find some use in perfume formulation where "leather" notes are desirable, as a modifier for Ethacol, Eugenol, Creosol and other phenolic ethers, and as a companion to Cade oil fractions, Birch Tar oil fractions, etc. and many chemicals used in achieving "leather" effect. Most of these chemicals, however, contain a free hydroxyl group in the benzene ring (a phenol group) which is not only active, but usually a source of much trouble for the perfumer (discoloration, etc.).

Prod.: Betelphenol which is the chief component of the natural Betel oil, can be produced synthetically from Methyl eugenol by treatment with Methyl Magnesium Iodide.

65-514; 68-974; 90-447;

## 348: BISABOLENE

*gamma*-Bisabolene.
A naturally occurring sesquiterpene, now available as a synthetic.



$C_{15}H_{24} = 204.36$

Colorless, slightly viscous oil, insoluble in water, soluble in alcohol, miscible with perfume oils. B.P. 262° C. Sp.Gr. 0.872.

Pleasant, warm, sweet-spicy-balsamic odor, inevitably reminding the perfumer of Opopanax and "Oriental" fragrance types.

Recently made available as a comparatively low-cost, pure and synthetic chemical (H.la-Roche Co.), this sesquiterpene should have a good and bright future in perfumery, not only as "another key material for some reconstituted essential oils", but also – and mostly – as a very attractive, colorless and stable material to form an important part of the fragrance picture of Oriental and Opopanax, Chypre, novelty fragrance types, etc.

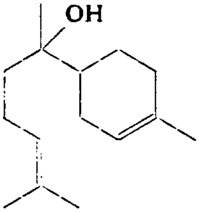
As mentioned above, it finds good use in artificial oils of Bergamot, Myrrh, Lemon, etc. and it is an excellent fixative for Neroli bases. It performs well in soap and acts as a stable fixative.

Prod. (several methods) e.g. from Nerolidol by dehydration.

65-84; 67-634; 87-231; (H.-laRoche info. sheet);

## 349: BISABOLOL

*alpha*-Bisabolol.



$C_{15}H_{26}O = 222.37$

Colorless viscous oil. B.P. approximately 265° C. Sp.Gr. 0.922.

Sweet and very mild, delicately floral odor.

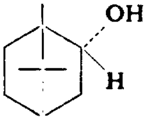
Although not regularly available or generally offered as a synthetic material yet, this sesquiterpene alcohol should soon become known and possibly find use as a blender/fixative of very versatile use. Its acceptability and popularity will, of course, largely depend upon the cost level. But with the enormous drop in the cost of synthetic Nerolidol over a period of less than 10 years to a level where this alcohol can be used in almost any type of fragrance, there may be good hope that Bisabolol can achieve a similar level of popularity.

Prod. via Nerolidol plus glacial Acetic acid with Sulfuric acid to yield Bisabolol acetate. Saponification of that ester yields Bisabolol.

88-245;

## 350: dextro-BORNEOL

Bornyl alcohol.
Borneo camphor.
*2*-Hydroxy camphane.
*d*-Camphanol.
*2*-Camphanol.
*2*-Hydroxy bornane.
*1*,*7*,*7*-Trimethyl bicyclo-*1*,*2*,*2*-heptanol-*2*.



$C_{10}H_{18}O = 154.25$

Hexagonal plates or leaflets. M.P. 204° C. B.P. 214° C. Sp.Gr. 1.01 (liquid).

Almost insoluble in water, poorly soluble in Propylene glycol, very soluble in alcohol, miscible with most perfume oils.

Dry-camphoraceous, woody-peppery odor. The dryness is characteristic and constitutes the main difference from the odor of *iso*-Borneol. The odor of Borneol is often compared to that of a good grade Rosemary oil (in which Borneol is present).

Borneol has a woody, somewhat minty and slightly burning taste.

This alcohol blends excellently with Olibanum products for "incense" type fragrances, and it forms a good background in many herbaceous-camphoraceous fragrances, Lavender- and Citrus cologne types, many types of Room-freshener fragrance, Pine odors, etc.

Borneol is used in Nut and Spice flavor compositions, usually in mere traces.

G.R.A.S. F.E.M.A. No.2157.

Prod.: by Sodium-reduction of *d*-Camphor. This yields a mixture of *d*-Borneol and *l*-*iso*-Borneol.

or by MPV reduction of Camphor. Yields 50/50 mixture of above.

or from Pinene via Pinene hydrochloride to Bornyl acetate to Borneol. Purification by dehydration to which Borneol is resistant.

NOTE: Although Borneol is classified as having a relatively low toxicity, it has a remarkable pharmacological effect upon many animals. It affects primarily the Central Nervous System.

4-23; 26-432; 65-239; 67-599; 85-37; 88-145ff; 88-168; 156-66; B-VI-75;

## 351: laevo-BORNEOL

Ngai camphor.

Structure and general synonyms: see *dextro*-Borneol. The common commercial Borneol is *dextro*-Borneol.

$C_{10}H_{18}O = 154.25$

Opaque (colorless) crystals. M.P. 208° C. B.P. 212° C.

Dry woody, slightly camphoraceous odor. Less peppery than *dextro*-Borneol.

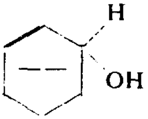
Rarely, if ever, offered (specifically *laevo*-) commercially, and probably of very limited interest to the creative perfumer or flavorist.

Prod. from *l*-Camphor which by reduction yields a mixture of *l*-Borneol and *d*-*iso*-Borneol.

Purification e.g. by dehydration, which acts fast upon *iso*-Borneol to yield Camphene, while Borneol is more resistant to dehydration.

65-239; 67-599; 88-145ff; 88-168; 100-162;

## 352 iso-BORNEOL



$C_{10}H_{18}O = 154.25$

White granular or flaky crystals. Softer than Borneol crystals, almost never "free flowing". M.P. 212° C. B.P. 214° C.

Insoluble in water, poorly soluble in Glycerin and Propylene glycol, very soluble in alcohol, soluble in most perfume oils.

Camphoraceous odor, not very woody, and not at all peppery. Overall more Camphor-like than Borneol.

Widely used in low-cost Pine fragrances (it is much less expensive than Borneol), Room spray fragrances, inexpensive Lavender, Fougere, and herbaceous type Colognes ,etc.

Occasionally used in flavor compositions, e.g. Fruit and Spice flavorings.

Concentrations are about 20 ppm in the finished product.

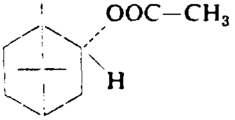
Prod. from Camphor or from Camphene. also: via Pinene-Camphene-(Acetylation)-*iso*-Bornyl acetate, and Saponification to *iso*-Borneol.

It is common, therefore, that the ester is less expensive than the alcohol (except for certain technical grades of *iso*-Borneol).

4-69; 7-220; 65-245; 67-599; 86-72; 88-177; 156-66;

## 353: laevo-**BORNYL ACETATE**

"Bornyl acetate".
(At one time called:
"Terpeneless Siberian Pine Needle oil").



$C_{12}H_{20}O_2$ = 196.29

Colorless liquid or crystalline mass, melting at 29° C. (when pure). (the inactive *dl*-form does not crystallize). Sp.Gr. 0.98. B.P. 226° C.

Very slightly soluble in water, almost insoluble in Propylene Glycol and Glycerin, soluble in alcohol and oils.

Sweet herbaceous-piney odor with a balsamic undertone. Reminiscent of Pine Needles.

Suggested for use in Fougeres, Chypres, Lavender colognes, Room spray fragrances, Bathoils, Pine fragrances, etc. Its odor is richer than that of the *iso*-Bornyl acetate.

Finds some use in flavor compositions for Fruit and Spice flavorings. The concentration will usually be about 70-80 ppm in the finished product.

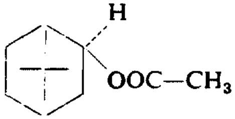
Prod. by esterification of *laevo*-Borneol. On account of its high melting point it can also be isolated from a mixture of isomers.

*dextro*-Bornyl acetate is produced from *dextro*-Borneol (esterification with Acetic anhydride and Sodium acetate).

G.R.A.S. F.E.M.A. No.2159.
FCC 1964-803.

4-24; 86-25; 100-162; 90-310;

## 354: iso-**BORNYL ACETATE**



$C_{12}H_{20}O_2$ = 196.29

Colorless slightly oily liquid. Sp.Gr. 0.98-0.99. B.P. 227° C.

Insoluble in water and Glycerin, poorly soluble in Propylene glycol, soluble in alcohol, Mineral oil and perfume oils.

Mild oily-piney, balsamic-camphoraceous odor, reminiscent of Spruce Needles or certain Pine Needles. The odor is overall thinner than that of Bornyl acetate.

Very extensively used in low-cost household fragrances, industrial fragrances, soap perfumes, masking odors, etc. It does not replace Bornyl acetate in "true-to-Nature" Pine Needle fragrance, but is generally accepted by the public consumer market as a Pine Needle fragrance material.

In blends with Terpinyl acetate, Coumarin and Amyl salicylate, it may form the basis of very low cost Fougere types.

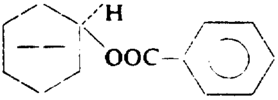
Used in some types of Fruit flavor. Concentrations in the finished product are usually about 10-15 ppm, but may run as high as 70 or 80 ppm in chewing gpm.

G.R.A.S. F.E.M.A. No.2160.
FCC-1964-839.

Prod. from Camphene (from *beta*-Pinene) by reaction with Acetic acid.

4-69; 45-503; 106-198; 156-70;

## 355: iso-BORNYL BENZOATE



$C_{17}H_{22}O_2 = 258.36$

Colorless viscous liquid. B.P. 320° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

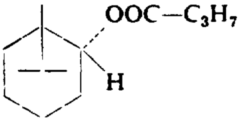
Very faint, sweet-piney or balsamic-piney odor of considerable tenacity.

This ester does not seem to offer any exceptional notes or effects and may never become more than a curiosity and find a place among thousands of research chemicals that failed to reach the perfumers' shelves.

86-25;

## 356: BORNYL BUTYRATE

*laevo*-Bornyl-*n*-butyrate.



$C_{14}H_{24}O_2 = 224.35$

Colorless liquid. Insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils. Sp.Gr. 0.97. B.P. 247° C.

Fruity-herbaceous, slightly woody-mossy odor, resembling the odor of herbal saps. Any trace of free Butyric acid, however, will completely destroy these unusual notes. Since this ester is comparatively rare, and rarely used, a sample on the perfumer's shelf may well be overaged, and should not be basis for evaluation of this ester.

Being an ester of Borneol, it is comparatively expensive and may not achieve great popularity as a perfume chemical. The *iso*-butyrate is less expensive and has a different odor, see next monograph.

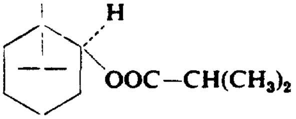
Prod. by esterification of Borneol.

4-24; 86-25; 156-70; 90-316;

## 357: iso-BORNYL-iso-BUTYRATE

(sometimes called Bornyl butyrate, commercially).

NOTE: *laevo*-Bornyl-*iso*-butyrate has been identified in natural oils.



$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. Insoluble in water, almost insoluble in Propylene glycol and Glycerin, soluble in alcohol and oils. Sp.Gr. 0.97. B.P. 239° C.

Peculiar earthy-nutlike, camphoraceous, fir-cone-like odor.

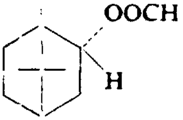
Suggested for use in perfume compositions, where its odor might fall well into the picture of low-cost Chypre, Fougere, Sage, etc. It is comparatively rare on the market and may well escape the noses of many perfumers. It is one of many chemicals that they probably would not lack in a whole life of practice.

Prod. by esterification of *iso*-Borneol.

43-734; 156-70;

## 358: BORNYL FORMATE

*laevo*-Bornyl formate.
(Also known in *dextro*-form).



$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. Almost insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils. Sp.Gr. 1.01. B.P. 215° C.

Somewhat green-earthy, yet refreshing odor with a pine-needle undertone.

Peculiar sweet taste, with a green-woody note.

This ester may be used in perfumes, but the author believes this is extremely rare.

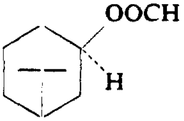
It is used in a few types of fruit flavors, usually in mere traces. The fresh-green odor and sweet-herbaceous taste is useful in fancy imitation Strawberry flavors and other fruit compositions.

G.R.A.S. F.E.M.A. No.2161.

Prod. from Borneol and Formic acid in the cold with acid catalyst.

4-24; 156-70; 90-301;

## 359: iso-BORNYL FORMATE



$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. Almost insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils. Sp.Gr. 1.01. B.P. 212° C.

Green-earthy, herbaceous-camphoraceous odor, more piney than that of the Bornyl formate, and more camphor-like, less nutlike.

Suggested for use in fruit flavors, and although this ester does have a sweet taste similar to that of Bornyl formate, it is overall less fruity or attractive.

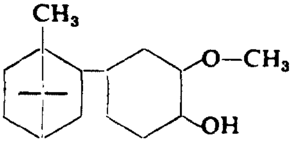
The use in fruit flavors amounts to a few ppm in the finished product (traces).

G.R.A.S. F.E.M.A. No.2162.

4-69; 7-220; 156-70;

## 360: iso-BORNYL METHOXY CYCLOHEXANOL

This material is the active odorous ingredient in various Sandalwood specialties, marketed under trade names.



$C_{17}H_{30}O_2 = 266.43$

Very viscous or syrupy colorless material, non-pourable at room temperature, consistency similar to that of honey. Insoluble in water, soluble in alcohol and oils.

Sp.Gr. 0.97 (commercial product).

The various specialties which contain this material as their chief ingredient, are usually made pourable by the addition of 10 to 30% of odorless oily solvent, sometimes with traces of Sandalwood terpenes or other additives. *iso*-Propylmyristate is one of several materials used for this purpose.

The commercial product has an extremely tenacious sweet-woody and slightly musky odor with considerable resemblance to Sandalwood. Some observers find animal notes, others find piney notes in the best known specialties. There is a considerable difference in odor between the various market products, based upon this chemical, but it can undoubtedly be said that the title chemical is the most successful Sandalwood type perfume chemical so far marketed. Its relatively low cost (about 25 to 35% of the Sandalwood oil price in 1966-1968) allows for extensive use in soap perfumes, and it is estimated that the annual world production is in excess of 100 tons, continuously increasing. Methods have been developed for identification of this chemical in Sandalwood oil, since panel tests have shown that additions of up to 20%, sometimes more, to natural Sandalwood oil, will not be detected in a perfume containing large proportions of Sandalwood oil by experienced consumer panels.

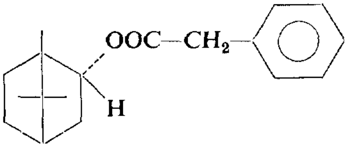
It is interesting to notice that the subject chemical is not at all chemically related to Santalol, the chief component of Sandalwood oil. There are opinions to the effect that Santalol is not responsible for the typical odor of that oil.

Prod.: (various methods) mostly starting from Guaiacol. However, it seems that the Guaiacol portion of the molecule of the subject material is *not* the deciding factor in the Sandalwood type odor.

See also:
*8-tertiary*-Butyl-*alpha*-benzosuberone.
*8-tertiary*-Butyl-*5*-methyl-*alpha*-tetralone.
*7-tertiary*-Butyl-*alpha*-tetralone-*1*.

## 361: BORNYL PHENYLACETATE

*laevo*-Bornyl phenylacetate.



$C_{18}H_{24}O_2 = 272.39$

Colorless viscous oil. Insoluble in water, soluble in alcohol and oils. B.P. 328° C.
Sp.Gr. 0.96.

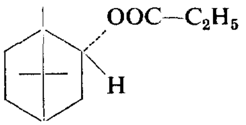
This ester is again one of those chemicals that have little more than academic interest and merely serve as a curiosity, if it appears on the perfumer's shelf at all.

The pure ester has very little odor, but could be used as a fixative. However, there are many better fixatives available at lower cost for the purposes that this ester could cover.

In combination with lower boiling perfume chemicals, this ester does contribute a perceptible note of floral-peppery character, but only at considerable concentration (and cost).

## 362: BORNYL PROPIONATE

*laevo*-Bornyl propionate.



$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid. Almost insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils.
Sp.Gr. 0.98. B.P. approximately 228° C.

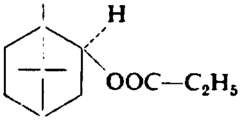
Warm-herbaceous odor, less piney and more Rosemary-Lanvandin-like than the acetate. Slightly fruity topnote. Helpful in building up Juniper-Cypress-like notes for Men's fragrances.

Suggested for use in Fougères, Chypres, Pine fragrances and many other non-floral types. As a modifier for Bornyl acetate, it lends a more versatile note and an overall desirable character to the fragrance. However, it cannot compete with the much less expensive *iso*-Bornyl propionate for general use in low-cost fragrances.

Prod. by esterification in the cold of Borneol with Propionic acid (plus acid catalyst).

156-70; 90-316;

## 363: iso-BORNYL PROPIONATE



$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid. Almost insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils.
Sp.Gr. 0.978. B.P. 245° C.

Sweeter, fruitier and less harsh than the acetate. The turpentine odor type is still there, but it is softer and combined with almost Lavender-like herbaceous notes.

Suggested for use in Fougères, Chypres, Pine fragrances, Citrus type Colognes, Lavender compositions for room sprays, etc.

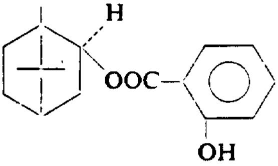
Traces of this ester are occasionally used in flavor compositions for imitation fruit, e.g. Strawberry, Blackcurrant, etc.

G.R.A.S. F.E.M.A. No.2163.

4-69; 43-622; 103-108;

## 364: iso-BORNYL SALICYLATE

**Note**: *dextro*-Bornyl salicylate is known as "Salit", and is described as "odorless".



$C_{17}H_{22}O_3 = 274.36$

Colorless viscous oil. Insoluble in water, soluble in alcohol and oils.

Very mild, delicately sweet-powdery odor of considerable tenacity.

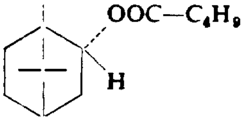
This material has been used as a sunscreening agent, and as such would enter cosmetic products at a significant level of concentration. Its odor is, however, in no way a disadvantage to its use, since it can be utilized in the fragrance type used in the cosmetic preparation.

The author doubts if this ester is used in perfumery as an odorant.

4-69; see also: 86-25;

## 365: BORNYL VALERATE

*laevo*-Bornyl-*n*-valerate.



$C_{15}H_{26}O_2 = 238.37$

Colorless liquid. Insoluble in water, almost insoluble in Propylene glycol and Glycerin, soluble in alcohol and oils. B.P. 249° C.
Sp.Gr. 0.96.

Fruity-herbaceous-camphoraceous odor, a herbal Pine type.

Sweet-herbaceous taste of considerable power.

This ester is used sparingly in various fruit flavors, and occasionally as part of special tobacco flavorings.

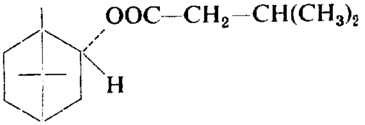
The author is not aware of any significant use of this ester in perfumery.

G.R.A.S. F.E.M.A. No.2164.

86-25; 156-70;

## 366: **BORNYL**-iso-**VALERATE**

*dextro*-Bornyl-*iso*-valerate.
"Bornyval" (Schering).
(The *laevo*-form is also known).



$C_{15}H_{26}O_2 = 238.37$

Colorless liquid. Insoluble in water, almost insoluble in Propylene glycol and Glycerin, soluble in alcohol and oils. Sp.Gr. 0.955. B.P. 260° C.

Although repeatedly described in literature as having the "odor and taste of Borneol and Valerian", this ester has, in the author's opinion, definitely an odor of its own, warm-herbaceous, slightly earthy-green, while the named off-odors probably derive from free – respectively Borneol and *iso*-Valeric acid in the partly decomposed ester. It is true that the slightest trace of free acid will completely ruin the original odor picture, but if such ester is tasted in aqueous solution, the effect of the acid again disappears and the true ester taste is perceptible.

Used in certain fruit flavor compositions, concentrations are but a few ppm (traces) in the finished product.

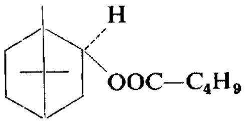
Prod. by esterification of Borneol with *iso*-Valeric acid (simple heating).

G.R.A.S. F.E.M.A. No.2165.

26-432; 90-319; 100-162; B-VI-162;

## 367: iso-**BORNYL VALERATE**

*dextro*-*iso*-Bornyl-*n*-valerate.



$C_{15}H_{26}O_2 = 238.37$

Colorless liquid, insoluble in water, almost insoluble in Propylene Glycol and Glycerin, soluble in alcohol and oils. B.P. 244° C. Sp.Gr. 0.95.

It is very conceivable that the user actually means *iso*-Bornyl-*iso*-valerate when this ester is mentioned. There is a considerable confusion in the use of the names of the four isomers.

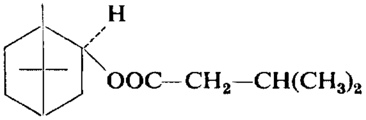
The author believes that this particular ester is the least common, perhaps never used.

Its odor is similar to that of the *iso*-valerate, but the ester is less stable than the *iso*-valerate, and therefore not preferred.

156-70;

## 368: iso-**BORNYL**-iso-**VALERATE**

(Often confused with *iso*-Bornyl valerate).
(See previous monograph).



$C_{15}H_{26}O_2 = 238.37$

Colorless liquid. Insoluble in water, almost insoluble in Propylene glycol and Glycerin, soluble in alcohol and oils.

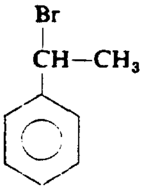
Herbaceous-camphoraceous, warm and slightly green-woody odor.

Used in certain types of fruit flavor, concentration in the finished product being only a few ppm (traces).

G.R.A.S. F.E.M.A. No.2166.

## 369: BROMO ETHYLBENZENE

*alpha*-Phenylethyl bromide.



$C_8H_9Br$ = 185.08

Almost colorless or pale yellowish mobile liquid. Insoluble in water, soluble in alcohol and oils.
B.P. approximately 200° C. (decompos.).
Sp.Gr. 1.31.

Peculiar warm-terpeney odor, remotely reminiscent of Pinus Pumilio or Juniperberry, also reminiscent of Lemon (terpenes).

Has been suggested for use in perfume compositions, but it is most conceivable that this chemical – like several others – with Bromine in its molecule (and in its name) cautions most perfumers from making use of it. Curiously enough, because the name Benzyl cyanide does not seem to scare nearly as many perfumers.

In any event, the author agrees that even the minimal possible hazard of free Bromine or Hydrobromic acid should be sufficient to eliminate this chemical from perfumers' shelves.

A pity, because the Juniper-like odor is extremely rare and has become increasingly popular in Men's fragrances in the late 1960's. Very few chemicals possess an odor of this type.

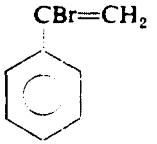
Prod. from Styrene and Hydrobromic acid.

NOTE: The *beta*-isomer is known. And so is *para*-Bromo ethylbenzene. None of them have interest to perfumers or flavorists.

4-24; 26-436; 68-957; B-V-355;

## 370: alpha-BROMOSTYROL

*alpha*-Bromostyrene.



$C_8H_7Br$ = 183.06

Pale yellowish mobile liquid. Almost insoluble in water, soluble in alcohol and oils.
B.P. approximately 190° C. (decompos.).

Pungent-sweet, gassy-floral odor, reminiscent of Hyacinth in extreme dilution. Slightly softer than the odor of *omega*-Bromostyrol.

Has been suggested as a modifier for the classic chemical *omega*-Bromostyrol, but does not seem to offer significant advantages.

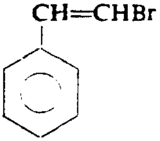
*alpha*-Bromostyrol is easily hydrolyzed in the presence of water or mild acid to Acetophenone (which will affect the odor type significantly).

Prod. from Styrene by treatment with Bromine. The resulting Styrene dibromide is treated with alcoholic KOH to yield *alpha*-Bromostyrol.

68-958; 86-26;

## 371: omega-BROMOSTYROL

*omega*-Bromo styrene.
*beta*-Bromostyrene.
Styryl bromide.
*1*-Bromo-*2*-phenylethylene.
"Hyacinthin".
*cis*- og *trans*-forms are known.
Commercial product is *trans-omega*-Bromostyrol.



$C_8H_7Br$ = 183.06

Pale yellowish mobile liquid. Almost insoluble in water, soluble in alcohol and oils.
Sp.Gr. 1.61 (NOTE). B.P. 219° C. (decompos.). Solidifies in the cold, melts at 7° C.

Very powerful, pungent-floral and somewhat gassy odor, in extreme dilution reminiscent of Hyacinth, with emphasis of the green-gassy pungency and very heavy sweetness. Poor tenacity.

This chemical, known for half a century, was once a very popular ingredient in soap perfumes. Its effect is similar to that of Phenylacetaldehyde, but gram for gram it is more powerful. However, the poor stability (and poor tenacity) of Bromostyrol puts it out of demand by modern perfumers. Traces of free Bromine or repulsive notes from Oxidation products (Bromo acetophenone, etc. – a teargas) are hazards of this chemical when not absolutely fresh and properly stored. It is claimed that the pure chemical is NOT an irritant to human skin.

Prod. from Cinnamic acid with Bromine in a non-polar solvent to yield Dibromo phenylpropionic acid, which is treated with aqueous Sodium carbonate to yield Bromostyrol.

The product is steam distilled out of the reaction mixture.

4-24; 5-10; 68-958; 86-26; 106-85; 95-195; 96-217;

## 372: BUTANE

$CH_3—CH_2—CH_2—CH_3$

$C_4H_8 = 58.12$

Colorless gas. Liquid below minus 0.5°C. Sp.Gr. (liquid) 0.58. The gas is twice as heavy as air. Flammable and explosive.

Sweet-ethereal, nauseating odor, perceptible only in relatively high concentration.

The gas is soluble at the rate of 12% (volume/volume) in water, and approximately 5% by weight in alcohol. It is miscible with most perfume and flavor oils, but does not dissolve many common resins, etc.

Butane is considered NOT toxic, but slightly narcotic. Its chief hazard is that of fire and explosion hazard.

It is used as a propellant in aerosol-dispensed consumer products, and it has been classified as G.R.A.S. by the American F.D.A. Accordingly, it may be used to a certain extent in food products, including those dispensed by aerosol (e. g. whipped "cream" etc.).

Prod.: from petroleum by distillation.

Butane is also isomerized to *iso*-Butane by heating with a metal halide catalyst. The *iso*-Butane is another important propellant in aerosol dispensers, but this isomer has not specifically been labelled G.R.A.S. by the American authorities. The isomer is an important gas and additive to motor fuel.

G.R.A.S. (classified as a food additive for miscellaneous use).

66-247; 100-176; 162-588;

## 373: 1,4-BUTANEDIOL DIVINYLETHER

$CH_2=CH—O—(CH_2)_4—O—CH=CH_2$

$C_8H_{14}O_2 = 142.20$

Colorless mobile liquid.

Insoluble in water, soluble in alcohol, miscible with oils.

Powerful, sweet-gassy, diffusive odor, in low concentration sweet and almost floral.

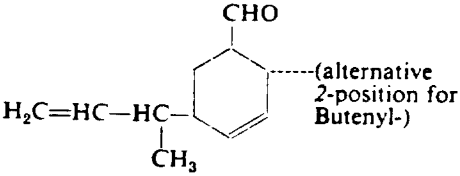
The title material which also serves as an intermediate in the manufacture of higher perfume chemicals, has found some use in perfume compositions, mainly for its diffusive power and "lift" in soap fragrances, detergent perfumes, etc.

It seems most conceivable that certain Vinylethers are the intermediate steps made by mother Nature in the manufacture (biosynthesis) of some very interesting and important odorous chemicals, including "Rose oxide". Many Pyran derivatives are made by means of Vinylether synthesis.

Prod.: from Tetramethylene glycol and Acetylene, using pressure and a catalyst.

## 374: 5-(or 2-)-(3-**BUTEN**-2-**YL**)-3-**CYCLOHEXENE CARBOXALDEHYDE**

*1,2,5,6*-Tetrahydro-*5*-(*3*-buten-*2*-yl)-benzaldehyde.
The commercial product consists most conceivably of the-*5*-isomer:



$C_{11}H_{16}O = 164.25$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Fresh, green-floral, delicately woody and quite tenacious odor.

This aldehyde is rarely offered under its proper chemical name, and it has not been very stable in the quality hitherto used.

It has been suggested for use in Muguet, Rose, Peony, Freesia, Magnolia and many other delicate or light floral fragrance types, where a discrete, green note is permissible.

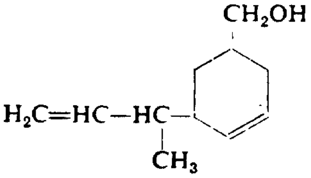
Chemically, it represents one of many results from a relatively new type of reaction in perfume chemistry. A number of useful perfume chemicals have come out of this type of research.

The corresponding alcohol, see next, and homologues have also found some use in perfumery.

Prod.: from Tetrahydrobenzaldehyde by condensation with Methyl vinyl carbinol (*3*-Buten-*2*-ol).

## 375: 5-(3-**BUTEN**-2-**YL**)-3-**CYCLOHEXENE METHANOL**

See previous monograph for possible isomers in commercial product.
*1,2,3,5*-Tetrahydro-*5*-(*3*-buten-*2*-yl)-benzyl-alcohol.



$C_{11}H_{18}O = 166.27$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral, slightly woody and winey-waxy odor of good tenacity.

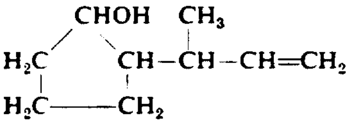
Occasionally offered under trade name, this alcohol has found some use in perfume compositions as a modifier in mild-floral and sweet-woody fragrance types, particularly in Rose, Mimosa, Peony, Magnolia, etc.

Its chemical name is of course not very attractive or easy to remember, and it is only reasonable to have a trade name which refers to the suggested use of the material.

Prod.: by controlled hydrogenation of the aldehyde (see previous monograph).

## 376: iso-**BUTENYL CYCLOPENTANOL**

*2*-(Methylvinylcarbinyl)-cyclopentan-*1*-ol.



$C_9H_{16}O = 140.23$

Colorless oily liquid. B.P. 190° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, herbaceous-floral odor of rather poor tenacity.

The title alcohol is used in perfume compositions, but is almost never found in price lists under its proper chemical name.

Its non-descript floral or floral-spicy or floral-herbaceous odor offers quite a variety of possibilities for this item.

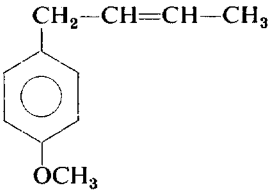
For those interested in the relationship between chemical structure and odor characteristics, a study of the material described in the previous monograph as compared to the item in this monograph, may be of some value.

Condensation products from Cyclopentanols and Cyclohexanols with alifatic or olefinic chains of 4 to 8 Carbon atoms have been thoroughly investigated during the past decade, and many interesting perfume materials have come out of that research.

Prod.: from Cyclopentenone and Methyl vinyl carbinol by condensation, followed by controlled hydrogenation to the secondary alcohol.

## 377: beta-BUTENYL-para-METHOXYBENZENE

4-(*2*-Butenyl)-methoxybenzene.
*4*-(*para*-Methoxyphenyl)-*2*-butene.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid. Insoluble in water, soluble in alcohol, miscible with oils.

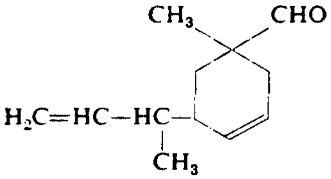
Intensely sweet, but also pungent-herbaceous-balsamic odor resembling the odor of Anise and Fennel, but with emphasis on the woody-herbaceous notes. Moderate tenacity.

This ether has been suggested for use in imitation Anise and Fennel oils, and for reinforcement of the said oils in perfume compositions. The author believes that the material is not used in flavors.

Prod. by Methylation of *para*-Butenylphenol.

3-286; 3-293;

## 378: 5-(3-BUTEN-2-YL)-1-METHYL-3-CYCLOHEXENE CARBOXALDEHYDE



$C_{12}H_{18}O = 178.28$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and delicate, fresh-green, mildly floral and woody odor of moderate tenacity.

Somewhat milder than its lower homologue (see above) this aldehyde has found some use in perfumery for its fresh-aldehydic and lightly floral notes, useful in Lilac, Lily, Muguet, Freesia, Rose, etc. It blends well with Cyclamenaldehyde, Hydroxycitronellal, Lilial, etc. all of which may benefit from the freshness of the title aldehyde.

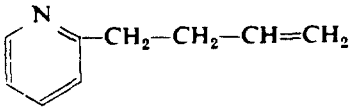
This is another material that almost needs a trade name to become popular. Perfumers would hardly be able to remember these chemical names, and certainly not willing to write such names down in their formula notebook every time they wanted to use some of these aldehydes and related chemicals. It has occasionally been offered under trade name but is not regularly available.

Prod.: from Cyclohexenone with Methyl magnesium bromide, followed by condensation with Methyl vinyl carbinol.

See also: *5*-(or *2*-)-(*3*-Buten-*2*-yl)-*3*-cyclohexene carboxaldehyde.

## 379: alpha-BUTENYL PYRIDINE

*2-(1-*Butenyl)-pyridine.



$C_9H_{11}N = 133.20$

Almost colorless, mobile oil. Insoluble in water, soluble in alcohol, miscible with oils.

Powerful and diffusive, gassy-green odor in dilution more foliage-green or vegetable green with an "earthy" bitterness, yet introducing a distinct sweetness of floral and also Fir-balsam character. This is another Pyridine derivative of potential interest to perfumery. It could find use as a trace component in top-note complexes with other "green" materials for novel effects, or in Geranium and Violet for "foliage" effect. Also in imitations of flower absolutes, e.g. Narcisse, Lily, Tuberose, and in fancy Pine fragrances.

See also: Butyl pyridine.

3-172; 3-189;

## 380: BUTTER ACIDS

Naturally occurring acids from Butter.

Although very far from being a well defined chemical this material has been included in the present work for the sake of completeness, and because Butter acids is considered a "flavor material". It is a mixture of:

Oleic acid, Palmitic acid – totalling 50 to 60% or even more.

Stearic acid, Myristic acid – totalling about 20% of "Butter acids".

Butyric acid – approximately 3 to 4% – being the highest amount of a low-alifatic acid.

Linoleic acid, Palmitoleic acid, Lauric acid, Caproic acid, Capric acid, Caprylic acid, and a number of other acids in amounts of less than one percent each. It is a waxy solid, low-melting product, poorly soluble in alcohol but soluble in oils and most flavor materials.

"Butter acids" is used in Butter and Cheese flavor compositions, usually in traces (a few ppm in the finished product), but the concentration in Butterscotch candy may be as high as 3000 ppm.

G.R.A.S.

107-211;

## 381: BUTTER ESTERS

Ethyl esters of the (mixed) acids from Butter. See previous monograph: "Butter acids".

The commercial product known as "Butter esters", usually contains a larger proportion of esters of the lower boiling acids, probably because "Butter esters" is usually a redistilled product.

Used in flavor compositions for Butter, Caramel, Chocolate and other imitation flavors.

Concentration is about 80 ppm in the finished product with above flavor types, but in special cases – such as Pop-Corn – the concentration may be as high as 1200 ppm.

G.R.A.S.

## 382: n-BUTYL ACETATE

$CH_3(CH_2)_3—OOC—CH_3$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Soluble 0.7% in water, soluble in Propylene glycol, miscible in alcohol and oils. B.P. 126° C. Sp.Gr. 0.88.

Very diffusive, etheral-fruity, pungent odor, reminiscent of many kinds of (ripe and over-ripe) fruit. Very poor tenacity. The odor is often described as resembling that of Pear, Banana, Strawberry, etc. but it may be closer to Pear than to any other single fruit.

Sweet-fruity taste in aqueous solution.

Used extensively in flavor compositions for imitation Apricot, Banana, Butter, Peach, Pear, Pineapple, Raspberry, Strawberry, etc.

Concentrations are usually about 30 to 35 ppm. In chewing gum it may amount to 200 to 240 ppm.

NOTE: This ester is flammable and its vapors form explosive mixture with air. *Fire hazard.* Flash point near room temperature.

Prod. by direct esterification of *n*-Butyl alcohol with Acetic acid or Acetic anhydride. Industrially by direct esterification in distillation column.

G.R.A.S. F.E.M.A. No.2174.

4-25; 26-440; 86-26; 100-177; B-II-130; 140-134;

## 383: iso-BUTYL ACETATE

$(CH_3)_2CH—CH_2—OOC—CH_3$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Soluble 0.66% in water, soluble in Propylene glycol, miscible with alcohol and oils. Sp.Gr. 0.871.
B.P. 116° C.

Very diffusive, ethereal odor resembling Rum ("fermented" odor) with a distinct fruity note.

Aqueous solutions have a sweet-fruity taste.

This ester is occasionally used in perfume compositions. Traces of the ester can introduce interesting lift and topnotes to delicate floral fragrances, such as Tearose.

Very commonly used in flavor compositions for its Banana-Pineapple-Raspberry-Pear-like notes. It finds use as a major ingredient in imitation Banana, Butter, Grape, Raspberry, Strawberry, and in "Tutti-frutti" types.

Concentrations are usually about 150-160 ppm in the finished product, but may amount to 800-900 ppm in chewing gum.

NOTE: This ester is highly flammable. Its flashpoint is at room temperature and its vapors form explosive mixtures with air. *Fire hazard.*

Prod. by direct esterification of *iso*-Butyl alcohol with Acetic acid or Acetic anhydride.

G.R.A.S. F.E.M.A. No.2175.

5-234; 26-440; 43-500; 44-806; 90-198; B-II-131; 100-571; 103-93; 140-134;

## 384: BUTYL ACETOACETATE

$CH_3(CH_2)_3—OOC—CH_2—CO—CH_3$

$C_8H_{14}O_3 = 158.20$

Colorless liquid. B.P. approximately 205° C.

Insoluble in water, soluble in alcohol and oils.

Sweet-winey, brandylike, "fermented-fruit"-like odor. Sweet and slightly fruity taste.

Used in various berry and fruit flavors, particularly for hard candy, etc.

Concentrations are usually about 25 ppm in the finished product.

Prod. by condensation of *n*-Butyl acetate plus Ethyl acetate, using Sodium ethoxide catalyst.

G.R.A.S. F.E.M.A. No.2176.

26-440;

## 385: iso-**BUTYL ACETOACETATE**

$(CH_3)_2CH—CH_2—OOC—CH_2—CO—CH_3$

$C_8H_{14}O_3 = 158.20$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. approximately 196° C.

Used in various berry and fruit flavor compositions, often as a modifier for the *n*-Butyl acetoacetate.

The odor is somewhat fresher, not as "fermented" as that of the *n*-Butylester, while the taste of the *iso*-Butylester is somewhat less sweet. In general, the former is preferred for "winey" effects, while this (latter) is preferred for fruity effects, and partly as a fixative for the more volatile esters used in hard candy flavoring etc.

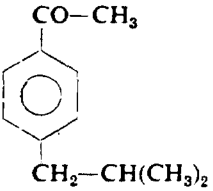
Concentrations are usually around 25 ppm.

Prod. by Claisen condensation of *iso*-Butyl acetate with Ethylacetate, using Sodium ethoxide catalyst.

G.R.A.S. F.E.M.A. No.2177.

## 386: para-iso-**BUTYL ACETOPHENONE**

"Homo Acetocumene".
Methyl-(*4-iso*-Butyl phenyl)-ketone.
*1*-Acetyl-*4*-*iso*-butylbenzene.



$C_{12}H_{16}O = 176.26$

Almost colorless liquid.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

The odor resembles that of *para*-Methyl acetophenone, but is somewhat milder, more refined, subdued. The character is more woody-hay-like, warm and quite tenacious.

This ketone has been suggested for use in perfume compositions to introduce herbaceous (or hay-like) notes in Mimosa, Violet, Lavender, Orris or versions of the "New Mown Hay" type.

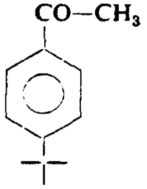
The title chemical is rarely offered by the regular suppliers of perfume chemicals.

Prod. (several methods) e.g. from Benzene, Acetyl chloride, *iso*-Butyl chloride (or -bromide) using Aluminium chloride catalyst in a Friedel-Craft type synthesis.

28-534; 86-72; 155-106;

## 387: para-tertiary-**BUTYL ACETOPHENONE**

"Alpha-iso-propyl Muguetton" (Jean A. du Crocq, Jr.).



$C_{12}H_{16}O = 176.26$

Colorless oily liquid. B.P. 232° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, very sweet, balsamic-floral, discretely herbaceous odor of moderate tenacity.

This ketone, which is related to an Ambre-smelling musk, also sold by the above company, has been commercially available for several decades, but is hardly ever offered under its proper chemical name.

It was originally meant to be a general floralizer for soap perfumes and cosmetic perfumes, since it is very stable and relatively inexpensive. Apparently it has not quite lived up to expectations, or it has had very hard competition from more modern perfume chemicals.

It is, however, still in use, and still considered a volume item.

It blends well with Cyclamen aldehyde, Terpineol, Tetrahydromuguol (IFF), the "rose alcohols", Styrax, etc.

It is interesting to notice the difference between this odor and the one of *para-iso*-Propyl acetophenone, see monograph: Acetocumene. See also monograph on *para*-Ethyl acetophenone, which is again different, but much closer related to the title material in odor type.

Prod.: from Benzene plus Acetylchloride and *tertiary*-Butylchloride with Aluminum chloride catalyst.

163-350; 163-378;

## 388: iso-BUTYL ACROLEIN

*beta-iso*-Heptenal.
*6*-Methylhexen-*2*-al-*1*.
(Exists in *cis*- and *trans*-forms).

$(CH_3)_2CH—CH_2—CH=CH—CHO$

$C_7H_{12}O = 112.17$

Colorless to pale straw colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Penetrating oily-green, vegetable-and-foliage type odor, in high dilution reminiscent of the odor of raw beans, green beans, etc., also of the odor of raw potatoes.

Has been suggested for use in perfume compositions as a modifier for other "green odor" chemicals.

However, this aldehyde is comparatively rare, and has probably found very little use in perfumery. It could find more use in flavor compositions for the increasingly interesting field of food flavoring and reconstitution of flavor in processed food. The concentration would probably be less than 1 ppm calculated on the finished product.

Prod. (several methods) e.g. by condensation of Acetaldehyde with *iso*-Butyric aldehyde.

3-169; 4-190;

## 389: n-BUTYL ALCOHOL

*1*-Butanol.
Butanol-*1*.
*n*-Propyl carbinol.

$CH_3—CH_2—CH_2—CH_2OH$

$C_4H_{10}O = 74.12$

Colorless, slightly oily liquid.

Soluble 9% in water, miscible with alcohol and oils. Sp.Gr. 0.81. B.P. 118° C.

Mild "fusel"-like odor, more volatile and more choking than fusel oil itself. Although somewhat winey in character, its odor is really nondescript, rather "chemical".

Used in flavor compositions for imitation Butter, Cream, Fruit, Liquor, Rum Whisky, etc.

Concentrations may be up to 35 ppm in the finished product.

Prod. (earlier isolated from fusel oil) (many methods) e.g.: Starting from Ethane via Ethanol to Acetaldehyde – Aldol – Crotonaldehyde and finally Butanol. Or by fermentation of Glycerin by selected bacillus.

G.R.A.S. F.E.M.A. No.2178.

26-440; 100-178; B-I-367; 87-458; 66-308;

## **390:** iso-**BUTYL ALCOHOL**

*primary iso*-Butanol.
*2*-Methyl-*1*-propanol.
*iso*-Propyl carbinol.
*1*-Hydroxymethyl propane.

$(CH_3)_2CH—CH_2OH$

$C_4H_{10}O = 74.12$

Colorless liquid. Soluble about 10% in water, miscible with alcohol and oils.
Sp.Gr. 0.81. B.P. 108° C.

Choking, cough-provoking odor unless diluted; then rather mild, chemical, sweet, yet somewhat harsh.

This is the main "Butylalcohol" in fusel oil.

Used in flavor compositions for imitation Butter, Cola, Fruit, Liquor, Rum, Whisky, etc.

Concentrations are usually not higher than 30 ppm in the finished product.

Prod. by isolation from Potato-fusel oil, or: by fermentation of certain Carbohydrates.

G.R.A.S. F.E.M.A. No.2179.

66-309; 87-459; 100-571; B-1-373;

## **391:** n-secondary-**BUTYL ALCOHOL**

*2*-Butanol.
*2*-Hydroxybutane.
Methyl ethyl carbinol.
Butylene hydrate.

$CH_3—CH_2—CH(OH)—CH_3$

$C_4H_{10}O = 74.12$

Colorless liquid. Soluble 8% in water, miscible with alcohol and oils. Sp.Gr. 0.81.
B.P. 99°,5 C.

Oily-vinous odor, sweeter than that of the *n-primary*-Butanol, and not as "fusel-oil"-like.

The author is not aware of any significant use of this alcohol in perfumes or flavors, but it is interesting to note that *secondary*-Butylalcohol has the lowest toxicity of all four isomers of Butylalcohol. Only for the sake of completion, all four alcohols are included in this work.

Prod.: by hydrogenation of Methyl ethyl ketone, or directly from petroleum gases, by hydration of Butylene.

66-309; 100-178; B-1-371;

## **392:** tertiary-**BUTYL ALCOHOL**

Trimethyl carbinol.
*2*-Methylpropanol-*2*.

$HO—C(CH_3)_3$

$C_4H_{10}O = 74.12$

Colorless liquid. Solidifies in the cold to an opaque mass, melting at 25°,6 C.
Miscible with water, alcohol and oils.
B.P. 83° C.

Camphoraceous and somewhat "minty" odor, the dryness being characteristic and different from the other isomers.

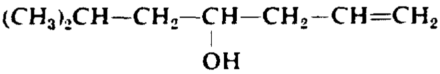
Has been suggested for use in perfume compositions, but its high vapor pressure makes it difficult to employ, except in certain types of industrial masking odors, where volatility may be desirable.

Prod. by hydration of *iso*-Butylene.

66-309; 100-178;

## 393: iso-BUTYL ALLYL CARBINOL

*alpha*-Allyl-*iso*-amylalcohol.
Allyl-*iso*-butylcarbinol.
*6,6*-Dimethyl-*1*-hexen-*4*-ol.
*6*-Methyl-*1*-hepten-*4*-ol.



$$(CH_3)_2CH-CH_2-\underset{OH}{CH}-CH_2-CH=CH_2$$

$$C_8H_{16}O = 128.22$$

Colorless oily liquid.

Powerful, woody-green somewhat oily odor, reminiscent of fresh woodsap and bark. At proper dilution, the woody notes become more minty-earthy, root-like, dry.

Has been suggested for use in perfume compositions as a modifier for other "green" chemicals, often in combination with Ionones, Vetiver oil, *iso*-Butylsalicylate, etc.

Prod.: (several methods) e.g.: from *iso*-Valeric aldehyde plus Allyl magnesium bromide by Grignard synthesis.

28-567; 155-106;

## 394: tertiary-BUTYL-tertiary-AMYL KETONE

*2,2*-Dimethyl-*4,4*-dimethyl hexan-*3*-one.
*2,2,4,4*-Tetramethylhexan-*3*-one.

$$(CH_3)_3C-CO-C(CH_3)_2CH_2-CH_3$$

$$C_{10}H_{20}O = 156.27$$

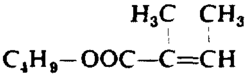
Occasionally mentioned in perfumery literature, and suggested for use in perfume compositions for its pronounced camphoraceous odor (which is rather typical of structures containing a *tertiary*-Butyl radicle).

However, there are many other and better chemicals for this olfactory purpose, and the author doubts if this particular one can ever become a standard item on the perfumer's shelf.

86-126;

## 395: n-BUTYL ANGELATE

*n*-Butyl-*cis*-*2*-methylcrotonate.
*n*-Butyl-*cis*-*2*-methylbutenoate.
*n*-Butyl-*cis*-*2,3*-dimethylacrylate.



$$C_4H_9-OOC-\overset{H_3C}{C}=\overset{CH_3}{CH}$$

$$C_9H_{16}O_2 = 156.23$$

Colorless liquid, almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, winey odor with distinct caramellic undertone.

Sweet-herbaceous taste, rather sharp in higher concentrations.

Finds some use in perfumery as a component of certain reconstituted essential oils. However, it seems beyond doubt, that it is the *iso*-Butyl angelate which occurs in (Roman) Chamomile oil. There is a slight odor difference between the two esters.

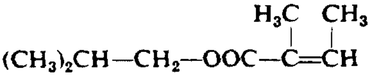
*n*-Butyl angelate could find use in flavor compositions, but since the *iso*-Butyl angelate – being a naturally occurring ester – has reached the safe place of the G.R.A.S. list, it is most conceivable that the *iso*-Butyl angelate will be the common ester of the two in the future.

Prod. by direct esterification of *n*-Butyl alcohol with Angelic acid.

NOTE: Commercial "Angelic" acid has – until recently – been a mixture of the two isomer acids: Angelic and Tiglic acid. Accordingly, the esters have been consisting of similar mixtures of two esters. Tiglic acid is the more stable form, and is more popular among the producers of the two acids.

## 396: iso-BUTYL ANGELATE

*iso*-Butyl-*cis*-2-methylcrotonate.
*iso*-Butyl-*cis*-2-methyl-2-butenoate.
*iso*-Butyl-*cis*-2,3-dimethylacrylate.



$$(CH_3)_2CH{-}CH_2{-}OOC{-}\overset{\overset{H_3C}{|}}{C}{=}\overset{\overset{CH_3}{|}}{CH}$$

$C_9H_{16}O_2 = 156.23$

Colorless liquid, almost insoluble in water, soluble in alcohol and oils. B.P. 177° C.

Fresh-herbaceous, winey-fruity odor, less warm, more fruity than the odor of the *n*-Butylester.

Being a very significant component of natural (Roman) Chamomile oil, and later identified in a great number of other essential oils, this ester has been known for a good many years. Contrary to what was once considered very unusual, the *iso*-Butylesters are not so uncommon in Nature.

Used in perfumery mainly as one of the "key" components in imitation Chamomile oil, but also as such to introduce unusual and generally desirable topnotes to novelty type fragrances.

Used in flavor compositions as a trace component in many types of flavors, fruit, wine, liqueur, Rum, etc.

The concentration in the finished product will usually be a few ppm only, except in icings where concentrations of this ester have been up to 100 ppm.

Prod. by direct esterification of *iso*-Butyl-alcohol with Angelic acid.

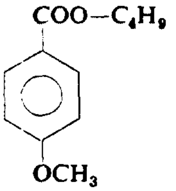
See NOTE – under previous monograph (*n*-Butyl angelate).

G.R.A.S. F.E.M.A. No.2180.

7-90; 66-311; 66-636; 90-221;

## 397: n-BUTYL ANISATE

*n*-Butyl-*para*-methoxybenzoate.



$C_{12}H_{16}O_3 = 208.26$

Colorless oily liquid. B.P. approximately 270° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, sweet and nondescript-floral odor, reminiscent of Mimosa, Cassie, and of the "dryout"-notes of heavy floral fragrances, e.g. Ylang-Ylang. It has good tenacity, but lacks character.

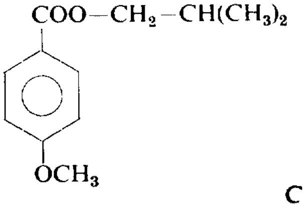
Suggested for use in perfume compositions as a blender-modifier-fixative in sweet-floral and "powdery" perfume types. It blends excellently with Ylang-Ylang, Cinnamic alcohol and Cinnamates, Benzyl salicylate, Nitromusks and non-Nitromusks, etc. But it does not seem to contribute much to a fragrance at concentrations below 3-5%. Being a comparatively rare chemical, it is not regarded as a "low-cost" item, and therefore not popular for high-percentage use.

Prod. by direct esterification of *n*-Butyl alcohol with Anisic acid under azeotropic conditions.

33-1138; 86-26;

## 398: iso-BUTYL ANISATE

*iso*-Butyl-*para*-methoxybenzoate.



$C_{12}H_{16}O_3 = 208.26$

Colorless oily liquid. Sp.Gr. 1.070.
B.P. approximately 255° C.

Faintly vinous, fruity-sweet odor with a rather heavy woody-floral undertone. It is characteristic of many odor descriptions of this type, that the word "Mimosa" or the word "Banana" appears. Curiously enough, Mimosa absolute is an interesting additive to artificial Banana flavor. This ester does have a Mimosa-type odor, and is used in flavors, including imitation Banana.

Useful in perfumes as a chemical with Mimosa-like effect – a most desirable variation of the old, repeated theme: Acetophenone-Methylacetophenone, etc. for Mimosa effect, these chemicals are, in the author's opinion, very far from the Mimosa type of odor.

*iso*-Butyl anisate blends well with all other heavy floral chemicals in Mimosa, Cassie, Ylang-Ylang, Peony, Gardenia, Carnation, Wallflower, etc.

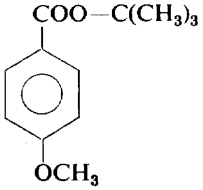
It is also used in flavor compositions outside of the U.S.A.

Prod. by direct esterification of *iso*-Butylalcohol with Anisic acid under azeotropic conditions.

34-681; 86-72; 103-113;

## 399: tertiary-BUTYL ANISATE

*tertiary*-Butyl-*para*-methoxybenzoate.



$C_{12}H_{16}O_3 = 208.26$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.04. B.P. approximately 300° C.

Faint, but heavy-woody-floral odor with an almost camphoraceous dryness. It is the least sweet of the three Butylanisates mentioned in this work.

This ester has been suggested for use in perfume compositions, but the author is convinced that it has little or no future in perfumery (or flavors). It does not contribute any highly desirable notes or very unusual notes that cannot be achieved by other, less expensive chemicals.

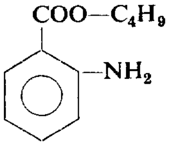
It is most conceivable that this ester came out of insecticide-research. Many derivatives of Anisic acid have such properties, and a great number of esters were made in search of pleasant smelling, effective insecticides.

Prod. by addition of *iso*-Butylene to Anisic acid.

33-1139; 86-125;

## 400: n-BUTYL ANTHRANILATE

*n*-Butyl-*ortho*-aminobenzoate.



$C_{11}H_{15}NO_2 = 193.25$

Colorless or very pale straw-colored liquid. Almost insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.07.

Mild, sweet-fruity-floral odor including the inevitable Orangeblossom theme, but overall flat and not as fresh in its type as the *iso*-Butylester.

Suggested for use in perfume compositions, mainly in Orangeblossom (as a modifier for lower homologues), Chypre, Oriental fragrances, Narcisse bases, etc.

The ester also finds use in flavor compositions for imitation Grape, Mandarin, Pineapple, Strawberry and Banana.

Being a comparatively powerful flavor chemical, it usually enters at concentrations around 10 ppm in the finished product.

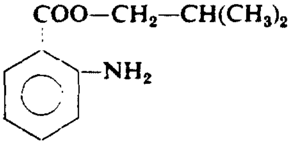
Prod. by direct esterification of *n*-Butylalcohol with Anthranilic acid under azeotropic conditions. Newer methods include the reaction of Isatoic anhydride with a Butoxide in alcoholic solution.

G.R.A.S. F.E.M.A. No.2181.

4-25; 77-213; 86-26; 103-113;

## 401: iso-BUTYL ANTHRANILATE

*iso*-Butyl-*ortho*-aminobenzoate.
*ortho*-Amino-*iso*-butylbenzoate.



$C_{11}H_{15}NO_2 = 193.25$

Colorless or very pale straw-colored liquid. Almost insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils. Sp.Gr. 1.06. B.P. approximately 270° C.

Pronounced fruity, very sweet and deep (warm) odor, yet fresh and with only a faintly floral undertone.

This ester, although known and used before many of today's perfumers were born, seemed to vanish from the shelves for several decades, until recently it had a renaissance in perfumes as well as in flavors.

It is an interesting modifier in Jasmin, Neroli and Orangeblossom fragrances, and lends tenacity, sweetness and richness to many types of floral or Oriental fragrances.

It is used quite extensively in flavor compositions, not only in the traditional Grape (American type) and Mandarin, but also in Cherry, Pineapple, Strawberry, Raspberry imitation flavors.

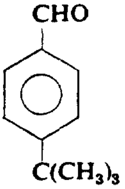
Concentrations are up to 12 or 14 ppm in the finished product, except in chewing gum where it may reach 1700 ppm.

Prod. by direct esterification of *iso*-Butylalcohol with Anthranilic acid under azeotropic conditions, or from Isatoic anhydride by reaction with e.g. Aluminium *iso*-Butoxide in *iso*-butylalcoholic solution.

G.R.A.S. F.E.M.A. No.2182.

4-69;

## 402: para-tertiary-BUTYL BENZALDEHYDE



$C_{11}H_{14}O = 162.23$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 246° C.

Warm-herbaceous, almost spicy odor of considerable tenacity.

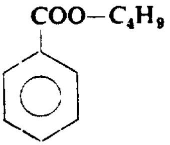
Has been suggested for use in perfume compositions as a modifier for Cuminic aldehyde which is so powerful that it causes difficulties in handling.

*para-tertiary*-Butylbenzaldehyde is milder and less green in its type than Cuminic aldehyde. However, it is a rare chemical, apparently not even offered from the regular producers of Cuminic aldehyde.

Prod. from *para-tertiary*-Butylphenyl magnesium bromide plus Ethyl-*ortho*-formate.

3-173; 68-515;

## 403: n-BUTYL BENZOATE



$C_{11}H_{14}O_2 = 178.23$

Colorless viscous liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils. B.P. 250° C. Sp.Gr. 1.01.

Very mild floral-balsamic odor with woody-spicy undertone.

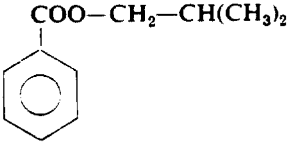
Useful in heavy florals with Ylang-Ylang, for Carnation, or as a blender-modifier-fixative or solvent with considerable tenacity and good stability against heat.

Prod. by direct esterification of *n*-Butylalcohol with Benzoic acid applying azeotropic conditions.

4-25; 26-442; 68-546; 100-179; 103-112; B-IX-112;

## 404: iso-BUTYL BENZOATE

"Eglantine" (This old name – of a Rose – is also applied to: *iso*-Butyl phenylacetate).



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid. Insoluble in water, miscible with alcohol and oils. Sp.Gr. 1.004. B.P. 242° C.

Weak, but fresh and pleasant, tenacious orrisy odor with green-rosy undertones, less balsamic than the *n*-Butylester.

Excellent fixative-blender for Orangeblossom, Orris and Violetbases, wild Rose, Sweet Pea, Acacia, Hyacinth, Ambre, etc. It seems to blend equally well with floral and non-floral compositions and it is an interesting companion for Labdanum products.

Used in flavor compositions for imitation Berry, Fruit, Cherry, Pineapple, Plum, etc.

Concentrations in finished product about 25 ppm.

Prod. by direct esterification of *iso*-Butyl alcohol with Benzoic acid, applying azeotropic conditions.

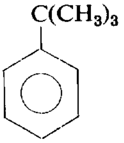
G.R.A.S. F.E.M.A. No.2185.

NOTE: The *n*-Butyl benzoate is NOT included in the G.R.A.S. list.

4-69; 26-442; 68-546; 103-112; 106-199; B-IX-113;

## 405: tertiary-BUTYL BENZOL

Pseudo butylbenzene.
Trimethyl phenylmethane.
*2*-Methyl-*2*-phenylpropane.



$C_{10}H_{14} = 134.22$

Colorless mobile liquid. Insoluble in water, soluble in alcohol and oils. B.P. 169° C. Sp.Gr. 0.867.

Peculiar camphoraceous-earthy, aromatic odor, remotely reminiscent of the odor of Carrot seed.

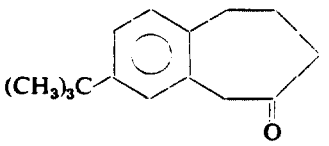
Has been suggested for use as a perfume chemical, but the author believes that there is very little, if any, use of this material in today's perfumery.

Prod. from Trimethyl pentane plus Benzene, using Aluminum chloride catalyst, or by a Friedel-Craft type reaction with *tertiary*-Butylchloride plus Benzene.

4-133; 66-243; 68-101; 68-110; 100-179; B-V-415;

## **406:** 8-tertiary-**BUTYL**-alpha-**BENZOSUBERONE**

*8-tertiary*-Butyl-*alpha*-benzo-cycloheptanone.



$C_{15}H_{20}O$ = 216.38

Colorless viscous liquid.

Peculiar woody odor, often described as reminiscent of Sandalwood (or burning Sandalwood) and therefore suggested for use in incense-type fragrances.

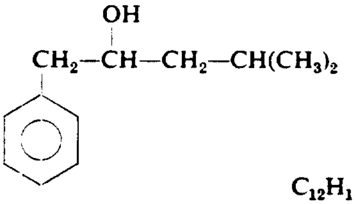
However, this chemical has not the versatility of more modern Sandalwood-chemicals, nor is it sufficiently close in odor type. It will probably remain a curiosity rather than a regularly used perfume chemical.

Prod. from *4-tertiary*-Butyl phenyl valeric acid plus Aluminum chloride.

9-70; 86-125;
See also:
*iso*-Bornyl methoxy cyclohexanol.
*8-tertiary*-Butyl-*5*-methyl-*alpha*-tetralone.
*7-tertiary*-Butyl-*alpha*-tetralone-*1*.

## **407:** iso-**BUTYL BENZYL CARBINOL**

Benzyl-*iso*-butylcarbinol.
*4*-Methyl-*1*-phenyl-*2*-pentanol.
*alpha*-*iso*-Butyl phenylethyl alcohol.
Benzyl-*iso*-amylalcohol.



$C_{12}H_{18}O$ = 178.28

Colorless, slightly oily liquid. Insoluble in water, miscible with alcohol and oils.
Sp.Gr. 0.96. B.P. 250° C.

Green-floral, fresh and slightly sweet-herbaceous odor, somewhat reminiscent of *iso*-Butyllinalool. Very good tenacity.

This carbinol, which is one of the highest boiling of the more common carbinols in perfumery, has found renewed popularity among perfumers after many years in oblivion. Apparently, its versatility has been discovered (or rediscovered?) by perfumers all over the world.

It is an excellent modifier in heavy and green floral fragrance types, in Oriental or Chypre bases, etc. It may form a significant basis of Honeysuckle, Freesia or variations of Rose or Muguet.

It is used in flavor compositions for imitation Butter, Caramel, Chocolate, Fruit and Spice in concentrations equivalent to 50 ppm in the finished consumer product.

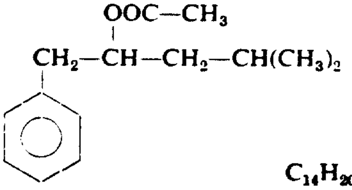
Prod. (several methods) e.g.: by Grignard reaction on Magnesium Benzyl chloride plus *iso*-Valeric acid, or: Phenyl acetaldehyde plus *iso*-Butylbromide.

G.R.A.S. F.E.M.A. No.2208.

86-72; 103-291; 156-76;

## **408:** iso-**BUTYL BENZYL CARBINYL ACETATE**

*alpha*-*iso*-Butyl phenylethyl acetate.
Benzyl-*iso*-butyl carbinyl acetate.



$C_{14}H_{20}O_2$ = 220.31

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

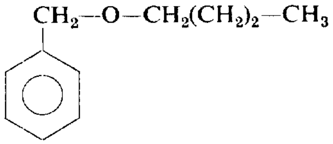
Fresh-floral, fruity and slightly green, natural-herbal odor. Good tenacity.

Used in perfumery for novelty fragrances, for special effects in delicate floral bases, Muguet, etc. and for modifications of Rose, Honeysuckle, etc. with or without the carbinol itself.

Prod. by direct esterification of the carbinol.

## 409: BUTYL BENZYL ETHER

Benzyl butyl ether.
Butyl benzyl oxide.
"Rose oxide" (*old* name).



$C_{11}H_{16}O = 164.25$

Colorless mobile liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.93.
B.P. 221° C.

Sweet floral, somewhat pungent odor, reminiscent of Rose and Geranium, but with a "chemical" note. In the description of the odor one often finds the word "metallic" which, in the author's opinion, is more appropriate for the Heptyl ethers.

Occasionally used in perfume compositions, mostly for soap fragrances, where the stability and power of this ether can be advantageous, or in industrial fragrances, low-cost detergent perfumes, etc.

Used in flavor compositions, mostly in fruit flavors.

Concentrations are rarely above 8 ppm in the finished product.

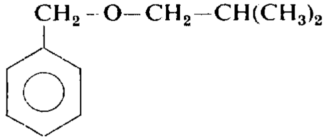
Prod. by dehydration of *n*-Butanol and Benzyl alcohol.

G.R.A.S. F.E.M.A. No.2139.

4-21; 4-25; 26-442; B-VI-410, (2' Ergänzungsband).

## 410: iso BUTYL BENZYL ETHER

Benzyl-*iso*-butylether.
Benzyl-*iso*-butyloxide.



$C_{11}H_{16}O = 164.25$

Colorless mobile liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.923.
B.P. 212° C.

Fresh-floral, somewhat "chemical", but overall sweet odor. Fresher and fruitier, but less rosy than the *n*-Butylether. Poor tenacity.

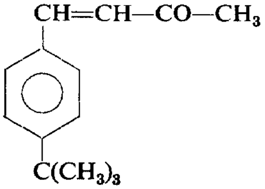
Occasionally used in soap perfumes for power, topnote (diffusion) and low cost. It is stable, but needs solid fixation in order to perform properly in soap. It blends excellently with Diphenyloxide and Diphenyl methane, both much higher boiling, and tends to take the harshness out of these chemicals.

Prod. from *iso*-Butylalcohol and Benzyl alcohol by dehydration.

4-22; 4-69;

## 411: para-tertiary-BUTYL BENZYLIDENE ACETONE

*4(para-tertiary*-Butyl-phenyl)-*3*-buten-*2*-one.
*para-tertiary*-Butyl benzalacetone.
*para-tertiary*-Butyl styryl methyl ketone.



$C_{14}H_{18}O = 202.30$

Yellowish oily liquid, solidifying in the cold to a crystalline mass of lemon-yellow color.

Heavy, sweet-herbaceous, somewhat spicy odor of good tenacity. Woody undertones.

Practically insoluble in water, soluble in alcohol, miscible with oils.

Suggested for use in perfume compositions, where its peculiar odor type may introduce new modifications of Fougere, Chypre, etc. or this chemical may be used to introduce a different type of fruitiness to novelty fragrances.

It blends well with Labdanum, Oakmoss, Patchouli, and with Amylsalicylate, Heliotropine, Coumarin, etc.

This ketone, like a great number of related ketones, has been suspected of being the cause of skin-irritation if used in more than trace amounts in the perfume. This may be one of the reasons why the title material has never achieved much popularity among perfumers.

Prod. from *para-tertiary*-Butylbenzaldehyde plus Acetone by condensation.

3-173; 4-195;

## 412: n-BUTYL-n-BUTYRATE

*n*-Butyric acid, *n*-butyl ester.
*n*-Butyl-*n*-butanoate.

$CH_3(CH_2)_3—OOC—(CH_2)_2CH_3$

$C_8H_{16}O_2 = 144.22$

Colorless, slightly oily liquid. 0.05% soluble in water, miscible with alcohol and oils. Sp.Gr. 0.870. B.P. 165° C.

Fresh and sweet-fruity, powerful and rather diffusive odor, reminiscent of Banana (overripe) and Pineapple.

Sweet and rich, fruity taste, pleasant in proper dilution.

Occasionally used in perfume compositions, mainly for special fruity notes in lipstick perfumes, or for modifying notes in novelty fragrances, where formerly Allyl caproate has been used in certain fragrance types.

Extensively used in flavor compositions for imitation Apple, Banana, Berry, Butter, Liquor, Peach, Pear, Pineapple, Nut, Scotch (whisky), Quince, etc.

Concentrations in the finished product are usually about 20 ppm, but may be as high as 1500 ppm in chewing gum ("Juicy-fruit"-type).

Prod. by direct esterification of *n*-Butyl alcohol with *n*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2186.

4-25; 26-442; 77-185; 86-26; 33-732; 90-204; 100-179; 103-113; B-II-271; 140-138;

## 413: n-BUTYL-iso-BUTYRATE

*iso*-Butyric acid, *n*-butyl ester.
*n*-Butyl-2-methyl propanoate.
This is the rarest of the 4 isomer esters.

$CH_3(CH_2)_3—OOC—CH(CH_3)_2$

$C_8H_{16}O_2 = 144.22$

Colorless liquid, almost insoluble in water, miscible with alcohol and oils. Sp.Gr. 0.862. B.P. 156° C.

Fresh-fruity, rather penetrating odor, reminiscent of Apple, Banana and Pineapple. Not as ethereal as the *iso*-Butyl-*n*-nutyrate.

Sweet fruity Banana-Pineapple like taste in aqueous media.

Occasionally used as a fruity modifier in lipstick perfumes.

Used in flavor compositions for imitation Apple, Apricot, Banana, Arak, Butter, Cherry, Ginger, Gooseberry, Hop, Melon, Blackberry, Orange, Peach, Pineapple, Raspberry, Strawberry, Tangerine, etc.

Concentrations in the finished product are normally about 40 ppm, except in chewing gum – up to 2000 ppm. (Juicy-fruit and Tuttifrutti type of flavors for chewing gum).

G.R.A.S. F.E.M.A. No.2188.

Prod. by direct esterification of *n*-Butyl alcohol with *iso*-Butyric acid under azeotropic conditions.

49-304; 86-27; 90-205;

## 414: iso-**BUTYL**-n-**BUTYRATE**

*n*-Butyric acid, *iso*-butyl ester.
*iso*-Butyl-*n*-butanoate.

$(CH_3)_2CH—CH_2—OOC—(CH_2)_2CH_3$

$C_8H_{16}O_2 = 144.22$

Sp.Gr. 0.865. B.P. 157° C.

Colorless liquid. Very slightly soluble in water, miscible with alcohol and oils.

Ethereal fruity, somewhat pungent odor reminiscent of Pear, Pineapple and Banana. Fresher, but not as soft as the *n*-Butyl-*n*-butyrate.

Sweet fruity taste in aqueous media.

Occasionally used in perfumery. One use is that as a masking agent for phenolic-cresylic type of undesirable odors.

Used in flavor compositions for imitation Apple, Banana, Berry, Liquor, Pear, Pineapple, Rum, etc.

Concentrations will normally be about 25 ppm in the finished product.

Prod. by direct esterification of *iso*-Butyl alcohol with *n*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2187.

4-70; 26-442; 33-732; 77-185; 103-113; B-II-271; 100-572; 140-138;

## 415: iso-**BUTYL**-iso-**BUTYRATE**

*iso*-Butyric acid, *iso*-butyl ester.
*iso*-Butyl-2-methyl propanoate.

$(CH_3)_2CH—CH_2—OOC—CH(CH_3)_2$

$C_8H_{16}O_2 = 144.22$

Colorless liquid. Insoluble in water, miscible with alcohol and oils. Sp.Gr. 0.875. B.P. 148° C.

Sweet-fruity, but also rather harsh-Pineapple-like, diffusive-ethereal odor. Fresher, but less characteristic (a non-descript fruit type) than the other isomers.

Occasionally used in masking odors for industrial masking of repulsive odors, phenolic, cresylic, "chemical" odors, solvent odors, etc. The relatively low boiling point (and high vapor pressure at room temperature) of this ester makes it particularly suitable for such purposes.

Used in flavor compositions for imitation Arak, Banana, Brandy, Butter, Fruit (Tutti-frutti), Liquor, etc.

Concentrations vary up to 15 or 18 ppm in the finished product.

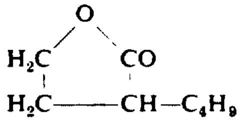
G.R.A.S. F.E.M.A. No.2189.

Prod. by direct esterification of *iso*-Butyl alcohol with *iso*-Butyric acid under azeotropic conditions.

4-70; 26-442; 33-732; 47-304; 86-73; 90-205; 100-572; 103-114; B-II-291;

## 416: alpha-n-**BUTYL**-gamma-**BUTYROLACTONE**

An isomer of Octalactone, this chemical is NOT identical with the one known as *gamma-iso*-Octalactone.



$C_8H_{14}O_2 = 142.20$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and most perfume and flavor materials. B.P. 230° C. Sp.Gr. 0.98.

Samples of subject material have shown considerable difference in odor, and the author is inclined to believe that other isomers are present in various proportions.

The classical odor picture: Cumin-Anise-Ambergris is rather vague, and does not really describe the material, be it pure or contaminated.

Leaving out Cumin and Anise, the Ambergris note may be perceptible to most observers, while the condiment-like or spicy sweet note resembles that of Caraway, although much softer with a Coconut-like background.

This lactone has been suggested for use in perfumes and flavors, but the author is not aware of any significant use of it in such products, nor does this lactone appear in price lists from regular suppliers of rare perfume and flavor chemicals.

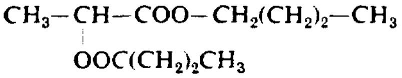
Prod. (many methods) e.g. from *n*-Butyl malonic ester plus Ethylene oxide.

30-254; 31-170; 86-26; 156-229;

This lactone is one of many prepared by Rothstein in the 1930's – still serving a purpose in research of correlation between odor and chemical structure.

## 417: BUTYL BUTYRYL LACTATE

Lactic acid, butyl ester, butyrate.



$$CH_3-\underset{\displaystyle OOC(CH_2)_2CH_3}{\underset{|}{CH}}-COO-CH_2(CH_2)_2-CH_3$$

$C_{11}H_{20}O_4 = 216.28$

Colorless to pale yellowish liquid. Slightly soluble in water, soluble in propylene glycol, alcohol and oils.

Sweet-sour "Buttermilk" type odor with a mild-fruity undertone. Not used in perfumery.

Used in flavor compositions for imitation Butter, Butterscotch, Fruit (including Tutti-frutti and the like), Nut, Vanilla and other flavors.

Concentrations vary up to 60 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2190.

Prod. by acylation-esterification of Lactic acid.

107-166;

## 418: BUTYL CAPRATE

Butyl decylate.
Butyl decanoate.
Butyl caprinate.

$(C_4H_9)—OOC(CH_2)_8CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol. B.P. 270° C. Sp.Gr. 0.870.

Heavy, oily-sweet, Brandy (Whisky-Cognac)-like odor with fruity topnote. Not very pleasant at high concentration. Odor resembles residue of Cognac or Whisky.

Rarely used in perfumery.

Used in flavor compositions for imitation Apricot, Brandy, Cognac, Wine, etc. – but this ester is NOT included in the G.R.A.S. list in the U.S. Federal Register.

It is most conceivable that the ester is used regularly in many other countries.

35-854; 86-26; 103-112;

## 419: n-BUTYL CAPROATE

*n*-Butyl hexanoate.
*n*-Butyl hexylate.

$CH_3(CH_2)_3—OOC(CH_2)_4CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. B.P. 208° C. Sp.Gr. 0.862.

Very slightly soluble in water, soluble in alcohol and oils.

Heavy vinous-fruity odor, reminiscent of overripe Pineapple, yet pleasant in high dilution.

Sweet fruity Pineapple-like taste in aqueous media.

Used in flavor compositions for imitation Butter, Pineapple, Rum, and in Butterscotch type flavor, etc.

Concentrations are usually about 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2201.

Prod. by direct esterification of *n*-Butyl alcohol with Caproic (hexanoic) acid under azeotropic conditions.

26-442; 33-733; 77-186; 103-112; B-II-323; 34-1230;

## 420: iso-BUTYL CAPROATE

*iso*-Butyl-*n*-hexoate.
*iso*-Butyl hexanoate.

$(CH_3)_2CH—CH_2—OOC—(CH_2)_4CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.86.

Heavy winey-fruity Pineapple-like odor. Fresher than the *n*-Butylester, and it displays, according to some observers, a Cocoa-like undertone.

This ester is occasionally used for special effects in Oriental fragrances, mainly as a modifier in the fruity complex and topnote.

It is used extensively in flavor compositions, primarily in imitation Pineapple, but also in Apple, Grape and other fruity types.

The concentration of this ester in the finished consumer product will normally be about 8 ppm.

G.R.A.S. F.E.M.A. No.2202.

Prod. by direct esterification of *iso*-Butanol with Caproic acid under azeotropic conditions.

4-70; 86-73; 106-200; 34-1230; 140-141;

## 421: n-BUTYL CAPRYLATE

*n*-Butyl octanoate.
*n*-Butyl octylate.

$(C_4H_9)—OOC(CH_2)_6CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless slightly oily liquid. B.P. 245° C. Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Fruity-green, slightly oily and floral. Refreshing fruity, slightly green taste.

Used in flavor compositions for imitation Apple, Cognac, Gooseberry, Wine, Pear, etc.

NOTE: This ester is NOT included in the U.S.A. "G.R.A.S."-list, but the material is used in many countries outside of the U.S.A.

Prod. by direct esterification of *n*-Butanol with Caprylic (*n*-Octanoic) acid under azeotropic conditions.

NOTE: Caprylic acid is also a common commercial name for 2-Ethyl hexanoic acid. It is most conceivable that the very contradictory odor/flavor descriptions of this ester in various publications may be due to the fact that there are esters of both acids sold under the name "Butyl caprylate".

4-25; 26-442; 33-733; 35-404; 86-23; B-III-348;

## 422: iso-BUTYL CAPRYLATE

*iso*-Butyl-*n*-octanoate.
*iso*-Butyl octylate.
Most commercial "Butyl caprylates" are *iso*-Butyl-.
NOTE: *iso*-Butyl-2-ethyl hexanoate is also called *iso*-Butyl caprylate commercially, and may cause some confusion and variations of odor description of the chemical under this name.

$(CH_3)_2CH—CH_2—OOC(CH_2)_6CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless oily liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Mild-herbaceous-woody, but overall fruity-oily odor with a faint, winey undertone.

Occasionally used in perfumes as a modifying fruity topnote in Oriental bases or as a new type fruity note in novelty fragrances.

Used in flavor compositions for Apricot, Cognac, Grape imitation flavors, etc.

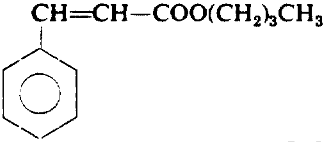
However, the chemical is NOT included in the American G.R.A.S. list.

Prod. by direct esterification of *iso*-Butanol with *n*-Octanoic acid.

4-70; 77-186;

## 423: n-BUTYL CINNAMATE

*n*-Butyl phenylacrylate.
"Eliminoxy" (Pharmaceutical name).



$C_6H_5—CH=CH—COO(CH_2)_3CH_3$

$C_{13}H_{16}O_2 = 204.27$

Colorless oily, or somewhat viscous, liquid. Like many other cinnamates, it tends to polymerize on standing and may turn hazy and more viscous. However, the Butylester seems less prone to polymerization than the Propylester. Sp.Gr. 1.012. B.P. 287° C.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol and Glycerin.

Sweet-oily-balsamic-fruity odor, remotely reminiscent of the odor of fresh Cocoa beans. Floral undertone and good tenacity.

Useful in perfumery where its unusual odor pattern can emphasize and improve the odor of Labdanum, it can mellow the sharpness of the odor of Eugenols, blends well with Ionones and woody odors, Lavender and Lavandin, etc. for Chypre and Ambre type fragrances.

The ester is used in flavor compositions mostly as a modifier for the Amylester, in imitation Chocolate, Cocoa, Fruit and Vanilla.

Concentrations are usually about 12-15 ppm in the finished product.

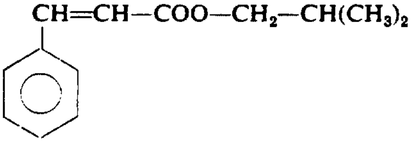
Prod. by direct esterification of *n*-Butanol with Cinnamic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2192.

4-25; 33-733; 86-26; 100-180; 77-195;

## 424: iso-BUTYL CINNAMATE

"Labdanol" (old French name).



$C_6H_5—CH=CH—COO—CH_2—CH(CH_3)_2$

$C_{13}H_{16}O_2 = 204.27$

Colorless, slightly viscous liquid.
Sp.Gr. 1.01. B.P. 271° C.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Herbaceous-balsamic odor with a faint, fruity undertone, warm and "Oriental" overall type. The overall odor pattern is also described as Ambre-Cocoa like, mild, sweet and tenacious, which however, more describes the use of this chemical.

It finds use in perfume compositions as a modifier/blender for Labdanum and other Ambre-type materials; it was in fact the "classical" Ambre-Labdanum chemical until more recently several Labdanum-smelling chemicals were developed (see Ethyl benzyl acetoacetate and Ethyl hydroxy phenylpropionate, also Ethyl benzoyl acetate).

The ester produces very attractive "powdery" notes with suitable fixatives and blenders, particularly musks, special Ionones, Patchouli oil, etc. – also for "Oriental" fragrance types.

Used in flavor compositions where it may introduce deep-sweet oily-fruity notes in imitation Chocolate, Cherry, Cocoa, Currant, Liquor, Peach, Plum Raspberry, Strawberry, etc.

The concentration of this ester in the finished consumer product is usually limited to mere traces (a few ppm).

Prod. by direct esterification of *iso*-Butanol with Cinnamic acid under azeotropic conditions.

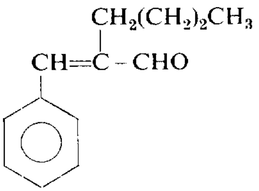
G.R.A.S. F.E.M.A. No.2193.

4-70; 5-268; 7-221; 7-233; 34-462; 72-134; 103-113; 106-201;

## 425: alpha-n-**BUTYL CINNAMIC ALDEHYDE**

Butylcinnamal.

*alpha-n*-Butyl-*beta*-phenylacrolein.



$C_{13}H_{16}O = 188.27$

Pale yellowish, oily liquid. Sp.Gr. 0.98.
B.P. 252° C.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Green-oily-herbaceous odor, usually with a floral undertone. The latter, however, seems to lack in certain shipments. The selection of fractions from vacuumdistillation of this product largely monitors the odor type of the composite product.

The aldehyde is used in perfumery – not very widely – as a modifier for the much more popular Amyl derivative, and the Hexyl derivative, both of which have milder, more versatile odors.

In flavor compositions, the aldehyde finds some use for imitation Fruit, Nut, Spice (cinnamon-types), partly as a fixative. Unless properly stabilized, the aldehyde will soon produce very unattractive off-notes, generally described as "rancid".

G.R.A.S. F.E.M.A. No.2191.

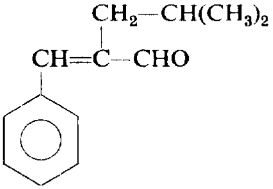
Prod. by condensation of *n*-Hexaldehyde with Benzaldehyde.

30-247; 156-28; 93-148/150;

## 426: alpha-iso-**BUTYL CINNAMIC ALDEHYDE**

*iso*-Butylcinnamal.

*alpha-iso*-Butyl-*beta*-phenylacrolein.



$C_{13}H_{16}O = 188.27$

Pale yellowish oily liquid. B.P. 257° C.
Sp.Gr. 0.98.

Rather penetrating, oily-fatty, herbaceous odor. There are variations in the odor type in lots from different suppliers, and in lots of different age.

Overall, the odor is less attractive than that of the *n*-Butylcinnamal.

The aldehyde has been suggested for use in perfume compositions as a modifier for the Amylcinnamal, but it is very doubtful if the *iso*-Butyl derivative will ever find application in perfumes. It does not contribute any unusual of very attractive notes to compositions.

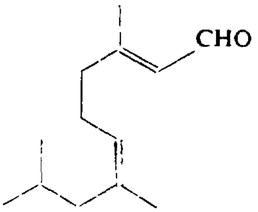
It may remain just a member of a long line of homologues of Amylcinnamal, developed in search of interesting derivatives.

Prod. from *beta-iso*-Propyl acetaldehyde (*iso*-Hexaldehyde) and Benzaldehyde by condensation.

93-150;

## 427: iso-BUTYL CITRAL

*3,7,9*-Trimethyl-*2,6*-decadien-*1*-al.



$C_{13}H_{22}O = 194.32$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 262° C.

Powerful and diffusive, waxy-fatty-floral odor, yet refreshing and natural odor. It is much sweeter and less lemony than Citral, and it has more of the natural Citral-Nerol character as for instance observed in Lemon Petitgrain oil, or in terpeneless Lemon oil.

The taste of this material is floral-lemony, but somewhat bitter in concentrations above 20 ppm.

After a decade of availability on the perfume chemical market and with a large and experienced manufacturer behind the promotion of it, this aldehyde has still not succeeded in obtaining a permanent space on the perfumer's shelf. In fact, it is simply missing from most perfume laboratories. The relatively high cost is probably one of the reasons.

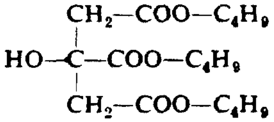
The title aldehyde could be used in fresh-floral compositions, such as Muguet, Lily, Ylang, and in many floral Citrus compositions, in "spring bouquet" fragrance types, etc. It adds a pleasant freshness to Hydroxycitronellal, and blends excellently with many carbinols.

Prod.: via *iso*-Butylheptenone and Grignard reaction with Ethoxy acetylene to an Acetylenic compound which is reduced and treated with weak hydrochloric acid to yield the subject aldehyde.

163-381;
(Hoffmann-laRoche sample).
The subject material is an isomer of Geranylpropionaldehyde and a lower homologue of Dihydro-nor-farnesal.

## 428: n-BUTYL CITRATE

Tributyl citrate.



$$\begin{array}{l} \qquad CH_2-COO-C_4H_9 \\ \qquad | \\ HO-C-COO-C_4H_9 \\ \qquad | \\ \qquad CH_2-COO-C_4H_9 \end{array}$$

$C_{18}H_{32}O_7 = 360.44$

Colorless liquid. Sp.Gr. 1.045
B.P. approximately 335° C.

Insoluble in water, soluble in alcohol and oils.

When absolutely pure, this ester has virtually no odor. However, a trace of Butanol-odor is often perceptible.

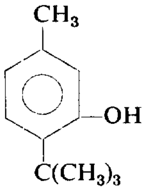
Butyl citrate has found some – but very little – use as a solvent/fixative in perfumes and flavors, but it can be classified as uninteresting to the creative perfumer or flavorist.

It has some interest from an academic point of view in the study of relationship between molecular weight and human olfactory perception.

Prod. by direct esterification of Butanol with Citric acid.

26-702; 49-472; 100-180; B-III-371-zweiter Ergänzungsband.

## **429:** para-tertiary-**BUTYL**-meta-**CRESOL**



$C_{11}H_{16}O = 164.15$

Colorless oily liquid. Solidifies in the cold. M.P. 23° C. P.B. approximately 230° C.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Dry-woody-leathery odor, usually described as "Russian Leather"-odor (Cuir de Russie). This term is very flexible however, and may refer more to the odor of the curing materials, rather than the actual odor of leather.

This phenol has been suggested for use in "Cuir" bases, in Colognes (particularly Men's fragrances) and as a "dry" note in novelty fragrance types.

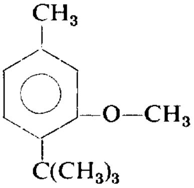
It is very powerful, but displays the same type of disadvantage as do other phenols: odor depression in alkaline media, therefore not recommended in soap, where it furthermore may cause discoloration.

Prod. from *iso*-Butylene plus *meta*-Cresol with Aluminium chloride.

31-23; 68-423;

## **430:** para-tertiary-**BUTYL**-meta-**CRESOL METHYLETHER**

Methyl-*4-tertiary*-butyl-*3*-methoxybenzene.



$C_{12}H_{18}O = 178.28$

Colorless or very pale yellowish liquid. B.P. 224° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, dry, Leather-like odor of moderate tenacity. The Leather-notes are different from those derived from various phenols, and approach the odor of the so-called "dephenolized Birch Tar Oil" to some extent.

This chemical has been suggested for use in "Cuir de Russie" type fragrances or other types of "Leather" odors, from time to time so popular, lately in the "Men's fragrance market".

The chemical was actually developed as an intermediate in the manufacture of Musk Ambrette, which is made by Nitration of subject material. The alkyl-substituted cresol-ether found some interest among the perfumers, and has been used ever since.

More leather-like odors have later been discovered among the Cyclohexane-derivatives, and it is most likely that subject chemical will soon vanish into oblivion in a file cabinet.

Prod.: from *meta*-Cresolmethylether plus *iso*-Butylchloride by condensation, using Aluminum chloride.

5-301; 28-584; 5-288;

## **431:** tertiary-**BUTYL**-iso-**CYANATE**

*tertiary*-Butyl carbimide.

$(CH_3)_3C-N=C=O$

$C_5H_9NO = 99.14$

Colorless liquid. B.P. approximately 100° C.

There is some confusion in the literature with respect to the odor of this chemical.

The author is of the opinion that it smells very unpleasant, pungent and that it is a lachrymator.

The unpleasant odor *could be* a result of formation of Butylamine as an intermediary product of the hydrolysis of the cyanate with moisture from the air. The cyanate is very sensitive to moisture (water).

However, when other authors describe the odor as "pleasant, floral, sweet, etc." it seems conceivable that a confusion exists with *tertiary*-Butyl-*iso-thiocyanate* (*tertiary*-Butyl mustard oil) which can be classified as sweet smelling. It is characteristic of "Mustard oils" with three or more Methylgroups as Alkyl-substitution that they are sweet smelling (2,4,6-Trimethyl-mustard oil = Mesityl-*iso*-thiocyanate is also sweet smelling).

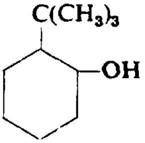
The subject cyanate has been included in this work in an attempt to enlighten the apparent problem of odor description.

Prod. from Potassium cyanate plus Di-*tertiary*-butylsulfate with Sodium carbonate in aqueous solution.

4-133; 4-193; 66-939; 86-143;

## 432: ortho-tertiary-**BUTYL CYCLOHEXANOL**

"Verdol" (I.F. & F.).



$C_{10}H_{20}O = 156.27$

Crystalline mass. Very slightly soluble in water, soluble in alcohol and oils.

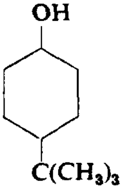
Powerful, camphoraceous-piney, mostly minty and somewhat tarry odor of great tenacity.

Being an isomer of the better known *para*-derivative, this alcohol is used in a similar way, mainly to lend power and radiation to soap perfumes where woody, Cedar-like, Pine-like or even Patchouli-like effects should be emphasized. Its minty character limits its use to a few fragrance types, and it will rarely enter the perfume formulation at more than one or two percent.

Prod. by hydrogenation of *2-tertiary*-Butylphenol.

## 433: para-tertiary-**BUTYL CYCLOHEXANOL**

"Padoryl" (Dow Chem. Co.).
"Patchone" (I.F. & F.).



$C_{10}H_{20}O = 156.27$

White powdery sublimate, needles or crystalline powder. Practically insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Extremely dry, woody-camphoraceous, almost "tarry" odor with a leather-like undertone.

Used in perfume compositions to lend power and diffusiveness to soap fragrances, along with woody notes, Ionones, Cedarwood oil derivatives, etc. and with the acetate of this alcohol. It is stable in soap and does not discolor in mixtures with any common perfume chemical.

Dating back to pre-war research in large German chemical companies, this alcohol remained practically unknown for some 15 years, then it was promoted as a "renforcateur" for Patchouli oil, or a key component in artificial Patchouli oil. It does not play this role any longer, but finds good use to impart lift and radiance to soap fragrances of the above types.

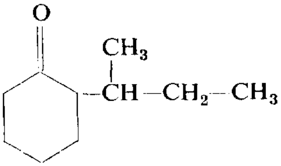
In late years it has found increased outlet in Lavandin blends where it gives interesting variations of the Borneol-*iso*-Borneol usage.

Prod. from *para-tertiary*-Butyl phenol by hydrogenation.

156-368;

## **434**: ortho-secondary-**BUTYL CYCLOHEXANONE**

An isomer of "Verdone" which is *ortho-tertiary*-Butyl-cyclohexanone (see next monograph).



$C_{10}H_{18}O = 154.25$

Colorless viscous liquid, solidifying to an opaque mass. Insoluble in water, soluble in alcohol, miscible with most oils.

Powerful and diffusive camphoraceous-woody, rather dry and musty odor of moderate tenacity.

This material, developed in search of new and interesting derivatives of Cyclohexanone along the manufacture of *para-tertiary*-Butyl cyclohexyl acetate, has not achieved any success worth mentioning in perfumery. Its odor type is much less desirable than that of its isomer (see next monograph), and even that remains a very restricted perfume chemical, because of its peculiar odor character.

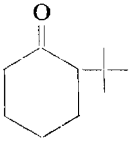
Apart from occasional use in soap and detergent fragrances, there is no real need for the title material.

Prod.: by hydrogenation of *2-secondary*-Butyl phenol.

NOTE: It may be of interest to those who study the relationship between chemical structures and olfactory characteristics, that the title material has the same emperical formula as Eucalyptol, and it has 2 Hydrogen-atoms more than Camphor, which it resembles more in odor.

## **435**: ortho-tertiary-**BUTYL CYCLOHEXANONE**

"Verdone" (I.F.F.).



$C_{10}H_{18}O = 154.25$

Opaque, crystalline, whitish mass, melting to a viscous, colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful and diffusive woody-camphoraceous and warm odor of moderate tenacity.

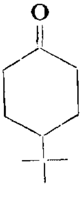
This material, although of very limited application in perfumery, can be used with some advantage in soap and detergent fragrances to increase the power and introduce more "lift" to the perfume. This is particularly noticeable in functional products which end up in hot water (detergents, etc.). The effect of Verdone is apparently enhanced by the heat and steam, since the material is quite volatile with steam, and it also sublimes when heated.

Prod.: by hydrogenation of *ortho-tertiary*-Butylphenol.

See also NOTE under previous monograph.

## **436**: para-tertiary-**BUTYL CYCLOHEXANONE**

"Product C-64" (Dow Chem. Co.).



$C_{10}H_{18}O = 154.25$

Colorless or white crystals. Almost insoluble in water, soluble in alcohol and oils. Sublimes under heating.

Powerful, dry-camphoraceous, slightly minty odor with woody Cedar-Patchouli-like undertones.

This material, commercially available for almost two decades, has only temporarily gained some importance as a powerful, "lifting" soap perfume ingredient, or as an inexpensive additive to Patchouli notes for soap and detergent fragrances, etc. It has more power and much less tenacity than Cedarwood and Patchouli, which is only an advantage in certain types of household products, where tenacity is not always very desirable.

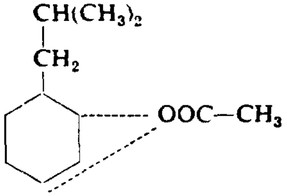
The title ketone can also give powerful "lift" to certain types of floral fragrance and to most of the herbaceous ones, Lavender, Lavandin, Rosemary, etc. It performs well with low-cost Fougere types along with Amylsalicylate and Ionones, and gives power to Pine fragrances. The corresponding secondary alcohol is a well-known perfume chemical ("Padoryl, Dow Chem. Co.) see No. 433 monograph.

The *ortho*-isomer is known, but it is of very little interest.

Prod.: by hydrogenation of *para-tertiary*-Butyl phenol. Complete hydrogenation yields "Padoryl", see No. 433 monograph.

## 437: iso-**BUTYLCYCLOHEXYLACETATE**

The commercial product was a mixture of *ortho-* and *para*-isomers (mainly) in an undisclosed proportion.



$C_{12}H_{22}O_2 = 198.31$

Colorless, slightly oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful fruity odor, remotely resembling Raspberry, but rather chemical and harsh at high concentration.

Very sweet, fruity taste, mainly Raspberry-type.

Suggested (by the producer) as a new flavor chemical and possibly a perfume chemical. However, it has not yet been approved for use in food in the U.S.A. In fact, very few Cyclohexanol-derivatives have been so approved. It is a pity, because there are now many interesting esters in the Cyclohexyl-methanol- and Cyclohexyl-ethanol- series that could be of great interest to the flavorist.

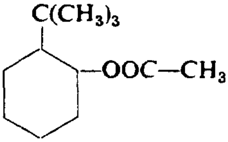
The series of Cyclohexanpropionates form an exception in that at least five of the higher and lower homologues of Allyl-cyclohexan propionate are approved for use in food flavors in the U.S.A.

Prod. by direct esterification of the alcohol (s).

ref.: Louis Hediger (deceased) in the "Trubek Distillate", 1959.

## 438: ortho-tertiary-**BUTYL CYCLOHEXYL ACETATE**

The acetate of "Verdol", see above.



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Almost insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

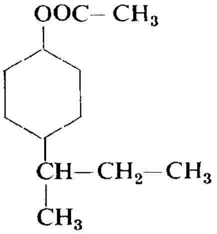
Piney-woody – fruity, powerful and fresh odor with a slightly green undertone. The power of this ester is often underestimated and can only be justly evaluated in actual use in perfume compositions.

Used as reinforcement for the fresh-piney, woody, Cedar-like notes in Pine fragrances for soap, household products, room sprays, etc. The fruity-green notes can be utilized in floral fragrance types, where this ester offers interesting modifications to the rather harsh and "thin" effect of Benzylacetate in Jasmin and other floral compositions.

Prod. by Acetylation of *2-tertiary*-Butyl cyclohexanol (Verdol).

## **439**: para-secondary-**BUTYL CYCLOHEXYL ACETATE**

An isomer of "Vertenex" –
see next monograph.



$C_{12}H_{22}O_2$ = 198.31

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Musty-dry, somewhat leathery-woody and Orris-like odor of moderate tenacity.

This ester, originally appearing as a minor component of the above mentioned isomer (see next monograph), has found very little application in perfumery. It is generally considered an undesirable type of odor, and it is virtually eliminated from the more popular isomer ester.

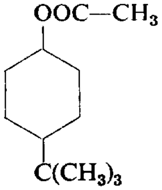
Prod.: by hydrogenation of *para-tertiary*-Butyl phenol to yield the alcohol from which the title ester is manufactured by conventional means.

## **440**: para-tertiary-**BUTYL CYCLOHEXYL ACETATE**

"Vertenex" (I.F. & F.).
"Vetester" (Arthol, Ltd.).
"Oryclon" (Haarmann & Reimer).
"Dorisyl" (formerly Dow Chem. Co.).
"Ylanat" (Dragoco).
"Phloxyl" (Naarden).
and many other specialty names.

The above commercial products are mixtures of *cis*- and *trans*-isomers of this ester, with or without trace components of chemically related Nature.

Usual proportion: Max. 70% *cis*-isomer, Min. 25-30% *trans*-isomer.



$C_{12}H_{22}O_2$ = 198.31

Colorless, slightly oily liquid. Sp.Gr. 0.936. B.P. approximately 232° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, almost "creamy"-woody odor with a soft-floral undertone, reminiscent of Ionones, Cedarwood and Benzyl salicylate. Some descriptions include the name Ylang-Ylang, but most perfumers agree that it is primarlily an Orris-type of odor.

Widely used in perfumery along with the Ionones, Cedarwood products, floral and non-floral perfume chemicals, a very versatile perfume material for soap and other low-cost fragrances, where volume is required. Generally as a blender/modifier in countless types of fragrances, from Pine to Rose, from woody to floral, it is one of the most successful perfume chemicals of the last few decades with respect to volume growth.

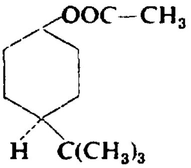
There is a considerable difference in the odor of the *cis*- and the *trans*-isomer ester, and the difference is pictured in esters from different suppliers. The *cis*-isomer is described in the next monograph. The *trans*-isomer is of little interest as such, but has been accepted up to a certain proportion partly influenced by the outcome of the hydrogenation process, partly forced by the available raw materials.

Prod. by Acetylation of *para-tertiary*-Butylcyclohexanol (made by hydrogenation of *para-tertiary*-Butylphenol).

156-368; 86-125; (also: manufacturers' data sheets).

## 441: cis-para-tertiary-BUTYL CYCLOHEXYL ACETATE

"Vertenex HC" (I.F. & F.).



$C_{12}H_{22}O_2 = 198.31$

Colorless slightly oily liquid. Almost insoluble in water, soluble in alcohol and oils.

The practically pure *cis*-isomer has a pronounced fruity note over the woody sweetness and velvety softness that make it resemble Orris products. It is interesting for the study of relationship between chemical structure and odor to note that the odor of the *cis*-isomer is not only distinctly different from that of the *trans*-isomer (dry, leathery, non-floral and weaker), but also that the *cis*-isomer resembles in odor the Trimethyl hexyl acetate (alifatic ester) to an amazing degree.

As the name from the above manufacturer implies, the product is claimed to have a Vetiver acetate-compatible odor, but the author finds that it does not nearly have the delicate and discrete approach to the human sense of smell, which is characteristic of Vetiver acetate, and for which reason the Vetiver acetate has been used as a major component in more than one very successful French fashion perfume.

This ester will, however, emphasize the clean, soft and slightly fruity notes in Vetiver, more so in the Methylionones, and it tends to sweeten Patchouli oil (of which certain lots are far from sweet).

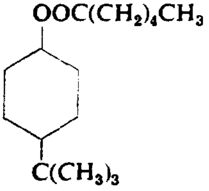
A recent process has brought a third quality of the ester on the market, stronger smelling than the regular grade, and with an odor more reminiscent of the Vetiver acetate-Vetiverol-Methylionone compositions, less fruity. (Vertenex Inter-*cis*, I.F.F.).

Prod. by Acetylation of the alcohol. A high-*cis*-content is achieved by hydrogenation with selected catalysts, and purification of the ester is improved by the fact that the *cis*-isomer distils somewhat lower than the *trans*-isomer.

156-368;

## 442: BUTYL CYCLOHEXYL CAPROATE

A mixture of *ortho-* and *para-tertiary*-Butyl cyclohexylhexanoate. (Originally an Agfa product).



$C_{16}H_{30}O_2 = 254.42$

Main component (*para*-isomer).
Colorless liquid, insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Mild, but rich and tenacious fruity-sweet odor with a Benzaldehyde-like undertone (impurity ? ?).

Has been suggested for use in perfumes and flavors when this ester first appeared in the late 1940's, parallel with many similar chemicals from the research department of Badische Anilin und Sodafabriken (B.A.S.F.) in Germany. However, it has not yet been approved for use in food in the U.S.A., and since it is not commonly offered to the creative perfume houses, this chemical has practically vanished from the shelves.

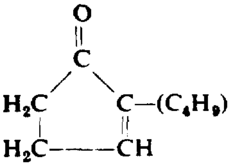
The *Allyl* cyclohexane *propionate* has achieved a reputation for interesting fruity Pineapple-type notes in perfumes and flavors (see the ester under that name).

Prod. from *(para)tertiary*-Butyl cyclohexanol by esterification with Caproic acid.

4-25; 86-26;

## 443: 2-BUTYL-2-CYCLOPENTENONE-1

(A lower homologue of Dihydro jasmone).



$C_9H_{14}O = 138.21$

Colorless or pale straw-yellowish liquid, slightly oily. Practically insoluble in water, soluble in alcohol and oils.

Sweet and warm, rather powerful floral odor of nondescript type, and with a perceptible woody-herbaceous undertone. A complex of generally pleasant notes.

Although this chemical is probably only one member of an almost endless line of Jasmone-research chemicals, it has been suggested as an interesting and individual odorant with possibilities in floral, Oriental and novelty fragrances. It s less sweet than Dihydrojasmone, somewhat more harsh (impurities??) and not nearly as versatile in actual use.

Very rarely offered commercially under its proper name.

4-25;

## 444: BUTYL-2-DECENOATE

*n*-Butyl decylenate.

$CH_3(CH_2)_2CH_2{-}OOC{-}CH{=}CH(CH_2)_6CH_3$

$C_{14}H_{26}O_2 = 226.36$

Colorless, slightly oily liquid.

Powerful, rich, oily-fatty, fruity odor, reminiscent of the peel section of Peach and Apricot. Natural-green undertones and moderate tenacity. Fruity-green, fresh and powerful taste. Used in flavor compositions for imitation Apricot and Peach, occasionally also Cherry and Plum or Mandarin.

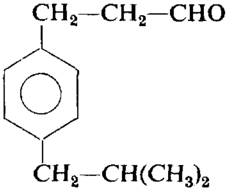
Concentration is usually about 35 ppm in the finished product, but in chewing gum it may reach 2000 ppm.

G.R.A.S. F.E.M.A. No.2194.

Prod. by direct esterification of *n*-Butanol with *2*-Decenoic acid.

## 445: iso-BUTYL DIHYDROCINNAMIC ALDEHYDE

*iso*-Butyl hydrocinnamic aldehyde.
*para-iso*-Butyl-*beta*-phenylpropionic aldehyde.



$C_{13}H_{18}O = 190.29$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

This aldehyde, also an intermediate in the manufacture of more interesting derivatives, has been suggested for use in perfume compositions as a floralizer and modifier of Cyclamen aldehyde and its homologues.

Its odor is mild, sweet, more balsamic than floral, and rather unnatural in its overall character.

The author suspects that mention of this aldehyde in perfumery literature could be confusing, and that the material most likely thought of in this connection is: *alpha*-Methyl-*para-iso*-butyl-hydrocinnamic aldehyde, see that monograph.

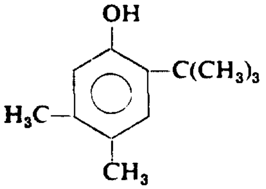
With a deficiency in power, and no truly natural floral character, there is not much future for the little aldehyde. It is rarely offered under its proper chemical name.

Prod.: from *iso*-Butyl benzaldehyde via *para-iso*-Butylcinnamic aldehyde, followed by catalytic hydrogenation.

127-157; see also Dr. P. Z. Bekoukian's annual report (1965) in the American Perfumer & Cosmetics.

## 446: ortho-tertiary-**BUTYL**-4,5-**DIMETHYL PHENOL**

*2-tertiary*-Butyl-*4,5*-dimethylphenol.



$C_{12}H_{18}O$ = 178.28

Colorless oily liquid, yellowish after exposure to air and daylight.

Slightly soluble in water, soluble in alcohol and oils.

Powerful, but not very pleasant "tanning" type of odor, sometimes describes as "Oak-moss-like" – at other times described as "Cuir de Russie" type. Most observers will agree that the odor is distinctly phenolic, very dry and almost woody, tarry.

There are many other – and better – odorants in this fragrance class and it is most likely that the subject phenol will remain a curiosity, not commercially available.

Prod. from *iso*-Butylene plus Xylenol, using Phosphoric acid as a condensing agent.

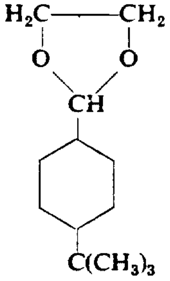
5-288;

## 447: 8-tertiary-**BUTYL**-1,4-**DIOXASPIRO**-4,5-**DECANE**

(Formerly a DOW aromatic chemical).

*para-tertiary*-Butyl cyclohexene carboxaldehyde ethyleneglycol acetal.

*2-(para-tertiary*-Butylphenyl)-*1,3*-dioxolan.



$C_{13}H_{24}O_2$ = 212.34

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Peculiar, somewhat animal, Skatole-like, woody odor in the Vetiver-Cedar type, with a chemical note. Not exactly pleasant in the pure state. It has some resemblance to the odor of certain Quinolines.

Suggested for use in perfumes, but apparently this chemical has been too difficult to employ, and it is most conceivable that it will never become a standard item. It has some interest for those studying the relationship between chemical structure and human olfactory perception.

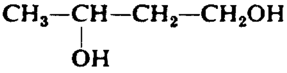
Prod. from the aldehyde with Ethylene glycol to yield a cyclic acetal.

## 448: 1,3-**BUTYLENE GLYCOL**

*1,3*-Butanediol.

*1,3*-Dihydroxybutane.

*beta*-Butyleneglycol.



$$CH_3-\underset{\displaystyle OH}{\underset{|}{CH}}-CH_2-CH_2OH$$

$C_4H_{10}O_2$ = 90.12

Colorless oily liquid. Sp.Gr. 1.00.
B.P. 207° C.

Miscible with water, soluble in alcohol and many perfume and flavor materials, but poorly soluble in hydrocarbons (terpenes, etc.).

Virtually odorless when pure.

Sweet taste with bitter aftertaste. The sweetness is perceptible only at high concentration (higher than 5000 ppm, while the bitter or metallic taste is perceptible at much lower levels.

However, at ordinary use-level, none of these taste impressions seem to interfere with the active aroma-components present (in solution or the like).

The title Glycol has achieved quite some importance as a flavor material solvent. It has certain advantages over Glycerine in its specific gravity being almost identical to that of water, it is inexpensive and commercially produced on a large scale.

The author believes, however, that Propylene glycol at the present time (1968) is still the leading solvent for flavor compositions.

Prod.: from Formaldehyde and Propylene under pressure and in presence of a catalyst.

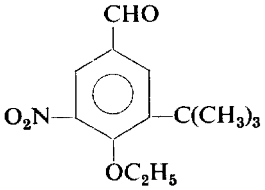
It has also been prepared from Aldol by reduction with Aluminum amalgam or by way of a catalyst.

G.R.A.S. (as a solvent for flavors). The material must be at least 99.00% *1,3*-Butyleneglycol.

66-475; 66-660; 162-590; B-I-477;

## 449: 3-tertiary-**BUTYL**-4-**ETHOXY**-5-**NITROBENZALDEHYDE**

This chemical is NOT identical to "Musk Aldehyde" (see 5-302).



$C_{13}H_{17}NO_4 = 237.28$

Pale yellowish or almost white crystalline powder. Insoluble in water, poorly soluble in alcohol, soluble in many perfume materials. Sweet musky, somewhat pungent odor.

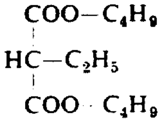
Has been suggested as a modifier to use along with the conventional Nitromusks. However, the subject Musk is less stable and more prone to discoloration that the common Nitromusks. It is therefore most conceivable that this Musk will remain practically unknown and unused.

Prod. from *3-tertiary*-Butyl-*para*-Ethylbenzaldehyde (1948).

48-294;

## 450: BUTYL ETHYLMALONATE

Ethylmalonic acid, Dibutylester.



$$\begin{array}{l} COO-C_4H_9 \\ HC-C_2H_5 \\ COO-C_4H_9 \end{array}$$

$C_{13}H_{24}O_4 = 244.34$

Colorless oily liquid, almost insoluble in water, soluble in alcohol, miscible with oils.

Decomposes upon heating to about 100° C.

Mild, oily-winey odor of moderate tenacity.

Fruity-winey, somewhat green-herbaceous taste in concentrations below 50 ppm.

This ester has been suggested for use in flavor compositions, partly as a blender/modifier, partly as a mild, fruity additive to various types of fruit imitation flavor.

Prod.: by condensation of Ethylbutyrate and Dibutyloxalate.

G.R.A.S.

## 451: iso-**BUTYL EVERNINATE**

***Everninic* acid, *iso*-Butylester.

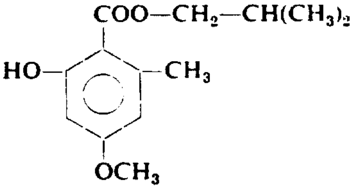
"*iso*-Butyl Lichenol".

*6*-Hydroxy-*4*-methoxy-*2*-methylbenzoic acid, *iso*-butylester.

*6*-Hydroxy-*4*-methoxy-*ortho*-toluic acid, *iso*-butylester.

*iso*-Butyl-*para*-methoxy orsellinate.

**Do not confuse with *Evernic* acid.



$C_{13}H_{18}O_4 = 238.29$

White crystals, needles, yellowish after exposure to air or daylight. Very slightly soluble in water, soluble in alcohol and oils, not in liquid paraffin.

Very dry, mossy, Oakmossy-phenolic odor, yet with considerable sweetness and excellent tenacity. Discolors upon exposure to daylight or air, and particularly in contact with alkali and iron.

Has been suggested for use in perfumery as a "colorless" Oakmoss chemical, but it still has the disadvantages of the conventional Oakmoss products, other than its own color.

Everninic and Evernic acid esters, the acids and the aldehydes are natural components, respectively breakdown products of Oakmosses and Lichens, but very few of these chemicals are commercially available yet.

The subject material is also used in artificial Vetiver oil.
4-70; 4-81;
See also: Ethyl everninate.
Methyl everninate.

## 452: n-BUTYL FORMATE

$CH_3(CH_2)_2CH_2—OOCH$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. Sp.Gr. 0.91.
B.P. 107° C.

Slightly soluble in water, miscible with alcohol and oils.

Very diffusive, ethereal, Rum-like odor. Volatile (very poor tenacity).

Sweet, Rum-Brandy-like taste in water.

Occasionally used as a topnote material in green-floral perfume bases. Used in flavor compositions for imitation Fruit (Tutti-frutti), Rum, Plum, Liquor and other flavors.

Concentration is usually about 10 to 12 ppm in the finished product.

Prod. by direct esterification of *n*-Butanol with Formic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2196.

26-444; B-II-21; 77-179; 86-26; 4-26; 103-83; 140-132;

## 453: iso-BUTYL FORMATE

Methyl-*iso*-propyl formate.
Tetryl formate.

$(CH_3)_2CH—CH_2—OOCH$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. 1 % soluble in water, miscible with alcohol and oils. Sp.Gr. 0.885. B.P. 98° C.

Mild-ethereal, pleasant odor, reminiscent of Rum and Raspberries, the "ethereal" odor arising from a barrel of Raspberries, freshly picked.

Sweet, fruity taste, but comparatively weak in aqueous solution.

Occasionally used as a modifier in fruity topnotes in novelty perfumes, it tends to further "lift" the topnote.

Used in flavor compositions, mainly in Raspberry and Rum, but also in other fruit flavor imitations, in Whisky flavor, Liquor, etc.

Concentrations are normally about 20 ppm in the finished product.

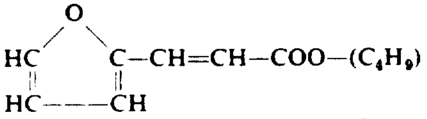
Prod. from *iso*-Butanol by direct esterification with formic acid under azeotropic conditions, using e. g. *para*-Tolylsulfonic acid catalyst.

G.R.A.S. F.E.M.A. No.2197.

C-1920-I-817; 4-70; 5-234; 26-444; 77-179; 103-84; B-II-21; 140-132;

## 454: BUTYL FURACRYLATE

*n*-Butyl furfuracrylate.
*n*-Butyl-*beta*-furylacrylate.
*n*-Butyl-*beta*-*2*-furanacrylate.
(Exists in *cis*- and *trans*-form, the commercial product being the *trans*-isomer).



$C_{11}H_{14}O_3 = 194.23$

Colorless or pale yellowish liquid.
Sp.Gr. 1.05. B.P. 248° C.

Insoluble in water, soluble in alcohol and oils.

Musty-floral odor, between the herbaceous and the floral, sweet and slightly green.

Herbaceous-winey, slightly spicy taste in concentrations below 20 ppm. Has been suggested for use in perfumes as a modifier in Fougères, Lavender compositions, etc., but is not regularly available, and has not achieved much interest among perfumers.

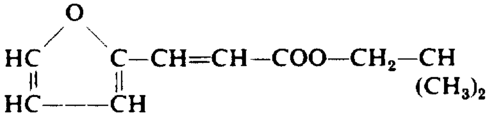
Could find some use in imitation Whisky, Brandy and similar flavors.

Prod. by esterification of *2*-Furacrylic acid with *n*-Butanol. The acid is obtained from Furfural by Perkins reaction.

3-297; 26-444; 86-26; 140-173;

## 455: iso-BUTYL FURACRYLATE

*iso*-Butyl-*2*-furanacrylate.
*iso*-Butyl-*beta*-*2*-furylacrylate.
*iso*-Butyl furfuracrylate.
(Exists in *cis*- and *trans*-form).



$C_{11}H_{14}O_3 = 194.23$

Colorless to pale yellowish liquid.
Sp.Gr. 1.02.

Insoluble in water, soluble in alcohol and oils.

Floral-herbaceous, sweet and somewhat cloverlike odor. Floral-herbaceous, slightly spicy taste.

Has been suggested for use in perfumery as a modifier in Fougeres, Lavenders, herbaceous-floral compositions, etc. However, the material is not regularly available, and it has some tendency to discolor (dark yellow).

Most conceivably, this chemical will remain a rare and infrequently used item.

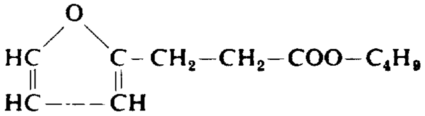
Has been suggested for use in imitation Brandy flavors.

Prod. by direct esterification of *2*-Furylacrylic acid, which can be obtained from Furfural by Perkins reaction.

140-173;

## 456: BUTYL FURFURHYDRACRYLATE

*beta*-Furyl propionic acid, *n*-Butylester.



$C_{11}H_{16}O_3 = 196.25$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar Brandy-like odor, woody-ethereal, not very tenacious. Sweet-spicy, rather nondescript taste.

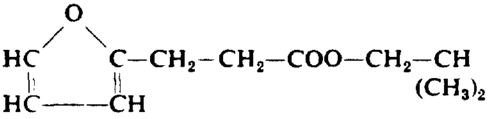
Suggested for use in flavor compositions, but is NOT included in the American G.R.A.S. list, although several closely related chemicals are so.

This chemical does not contribute any specific notes that are not obtainable with other materials, and it is a comparatively rare item.

3-23; 4-26; see also: 77-197; 140-174;

## 457: iso-BUTYL FURFURHYDRACRYLATE

*iso*-Butyl furylpropionate.
Commercially often called:
Butyl furfurhydracrylate (see previous monograph).



$C_{11}H_{16}O_3$ = 196.25

Colorless or pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Fruity-winey, Brandy-like odor with bitter-woody undertones and moderate tenacity.

The taste is pungent unless concentration is lower than 50 ppm, dry-fruity, Brandy-like, sweet and slightly spicy at concentrations near 10 ppm.

This ester has been used in flavor compositions where fruity notes are combined with Nut-like or "pit-like" notes, e. g. Peach, Plum, Cherry, Almond, etc. but the use of this ester has been abandoned in most countries.

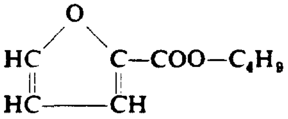
There is considerable confusion with respect to the nomenclature of the Furfural derivatives, particularly the esters of the alkyl-substituted Furanacids. This fact may have contributed to the lack of interest and to the reluctance in using these materials on the part of the new generation of flavorists.

Prod.: by esterification of *2*-Furanpropionic acid with *iso*-Butanol.

See also previous monograph.

## 458: n-BUTYL FUROATE

Furan-*alpha*-carboxylic acid, *n*-Butylester.
*n*-Butyl pyromucate.
*n*-Butyl-*2*-furoate.



$C_9H_{12}O_3$ = 168.20

Colorless liquid. Sp.Gr. 1.06.
B.P. approximately 216° C.

Insoluble in water, soluble in alcohol and oils.

Brandy-like, sweet, somewhat "burnt" odor with a woody note. Sweet-winey taste.

Suggested for use in flavor compositions as a modifier in Whisky-Brandy-Rum-Arak imitation flavors.

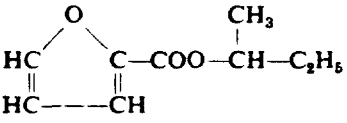
This ester is NOT included in the American G.R.A.S. list among chemicals permitted for use in food flavorings.

Prod. from *n*-Butanol and Furan-*2*-carboxylic acid by direct esterification. The acid is obtained from Furfural by Oxidation or by Canizzaro reaction.

3-22; 4-24; 26-444; 140-174;

## 459: secondary-BUTYL FUROATE

Methyl ethyl carbinyl furan-*2*-carboxylate.
Methyl ethyl carbinyl pyromucate.



$C_9H_{12}O_3$ = 168.20

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Winey-Brandy-like odor, more woody, somewhat chemical and not as pleasant as the *n*-Butylester.

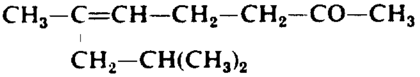
Rarely offered commercially, this ester – intended for use in flavor compositions – has little or no future as a flavor chemical. NOT approved for food in U.S.A., and not really offering unique effects, it will remain just a member of a long line of research chemicals, esters of Pyromucic acid and its homologues.

Prod. by direct esterification of *secondary*-Butanol with Furan-*2*-carboxylic acid.

See also the *n*-Butyl ester, previous monograph.

## 460: iso-BUTYL HEPTENONE

*6-iso*-Butyl-*5*-hepten-*2*-one.
*6,8*-Dimethyl-*5*-nonen-*2*-one.



$$\begin{array}{l} CH_3-\underset{|}{C}{=}CH-CH_2-CH_2-CO-CH_3 \\ \qquad CH_2-CH(CH_3)_2 \end{array}$$

$C_{11}H_{20}O = 168.28$

Colorless slightly oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful fatty-green, floral and sweet odor with fruity undertones. Moderate to good tenacity.

Used in perfume compositions as a powerful and interesting modifier in Fougères, where the green and the floral notes fall in place. As a modifier for *iso*-Butyl linalool in certain florals, such as Gardenia, Orangeblossom, etc.

Prod.: from Methyl-*iso*-butyl ketone plus Acetylene, via the acetylenic alcohol to *iso*-Butyl butenol, followed by ketonization with Diketene to the title material.

info.: Hoffmann-laRoche, Inc.

## 461: iso-BUTYL HEPTIN CARBONATE

*iso*-Butyl octynoate.
*iso*-Butyl hept-*1*-yne-*1*-carboxylate.

$(CH_3)_2CH-CH_2-OOC-C\equiv C(CH_2)_4CH_3$

$C_{12}H_{20}O_2 = 196.19$

Colorless oily liquid. B.P. 235° C.

Powerful, but relatively pleasant violet-green odor. Less fatty than the Methylester, not as pungent.

Suggested for use in perfume compositions as a modifier for other (lower) homologues of the series. It seems however, that beyond the Methylesters, it is the Amyl esters that have managed to maintain some interest. The Amylester of above series is generally considered superior as a fragrance material.

Its use is therefore very limited – in a few Violet bases, Narcisse, Hyacinth and other green-floral bases.

Prod. from Sodium heptyne (obtained from Castor oil) plus *iso*-Butyl chloroformate.

5-245;

## 462. n-BUTYL HEPTOATE

*n*-Butyl heptanoate.
Butyl heptylate.

$CH_3(CH_2)_2CH_2-OOC(CH_2)_5CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless, slightly oily liquid. Sp.Gr. 0.87. B.P. 225° C.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, fruity-green, Apple-peel like (unripe Apple) odor, also described as "Marigold"-like.

Sweet green, fruity taste.

Used in flavor compositions for imitation Apple, Coconut, Ginger, Hop (Beer), Fruit, Liquor, Plum and other flavors.

Concentrations are usually about 25 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2199.

Prod. by direct esterification of *n*-Butanol with *n*-Heptanoic acid.

4-26; 33-733; 86-27; 103-112;

## 463. iso-BUTYL HEPTOATE

*iso*-Butyl heptanoate.
*iso*-Butyl heptylate.

$(CH_3)_2CH—CH_2—OOC(CH_2)_5CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless, slightly oily liquid.

Insoluble in water, soluble in alcohol and oils.

Fruity-winey, fresh odor, not as green as that of the *n*-Butylester.

Sweet fruity-brandylike taste.

Used in flavor compositions for imitation Brandy, Cognac, Fruit (Tutti-frutti) and various Liquor flavorings.

Concentrations are usually about 25 ppm in the finished product but may be much less in flavored products where this ester is only a modifier in the flavor composition.

Prod. by direct esterification of *iso*-Butanol with *n*-Heptanoic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2200.

4-70;

## 464. n-BUTYL HEPTYL ETHER

Heptyl butyl ether.
Heptyl butyl oxide.

$C_4H_9—O—C_7H_{15}$

$C_{11}H_{24}O = 172.31$

Colorless mobile liquid. B.P. 205° C.
Sp.Gr. 0.79.

Insoluble in water, soluble in alcohol and oils.

Green-buttery, slightly "metallic"-chemical odor. The buttery note may be caused by the presence of traces of oxidized *n*-Butanol. This chemical is mostly available from producers of large-volume Petrochemicals or industrial chemicals, rarely made by the manufacturers of perfume chemicals. The standard quality therefore, may not be the most desirable odor from a perfumer's point of view.

Suggested for use in perfume compositions, but has hardly found outlets, except perhaps in certain masking odors and fragrances for industrial purposes, where power and low cost are important. Trace amounts may be used in certain artificial essential oils, where many peculiar fragrance notes are called for.

Prod. by dehydration of *n*-Butanol and *1*-Heptanol.

4-26;

## 465. iso-BUTYL HEPTYL ETHER

*n*-Heptyl-*iso*-butylether.
*iso*-Butyl heptyl oxide.

$(CH_3)_2CH—CH_2—O—C_7H_{15}$

$C_{11}H_{24}O = 172.31$

Colorless liquid. B.P. 194° C.
Sp.Gr. 0.79.

Insoluble in water, soluble in alcohol and oils.

Slightly green, woody-floral, somewhat chemical-metallic odor, remotely reminiscent of topnotes in Bois de Rose or Lavender. It bears some resemblance to the odor of "poor grade" Linalool (old-fashioned Bois-de-Rose-Linalool).

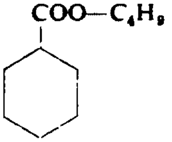
Apart from some interest to the student of chemical structure correlation with substance odor, this chemical has been used now and then in Fougeres and Lavender compositions as part of the reinforcing notes to the Lavender or Linalool theme. It blends well with these materials and with Amylsalicylate, *iso*-Butylsalicylate, Cedarwood derivatives, etc. However, its use in perfumery is very limited.

Prod. by dehydration of *iso*-Butanol and *1*-Heptanol.

4-70;

## 466. BUTYL HEXAHYDROBENZOATE

*n*-Butyl cyclohexanecarboxylate.



$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Powerful, warm-aromatic odor with a peculiar complex of rather unnatural notes, slightly woody-fruity, but not entirely pleasant.

This ester has been suggested for use in perfume compositions mainly as a powerful and relatively stable odorant in low-cost soap and detergent fragrances, but it has not achieved any popularity, and it is not regularly available from the normal suppliers of perfume chemicals.

Prod. by esterification of Cyclohexane carboxylic acid. The acid is obtained by catalytic hydrogenation of Benzoic acid.

## 467: BUTYL HEXYL KETONE

5-Undecanone.
*n*-Hexyl-*n*-butylketone.
Undecan-5-one.

$C_4H_9—CO—C_6H_{11}$

$C_{11}H_{20}O = 168.28$

Colorless oily liquid. Solidifies in the cold to an opaque mass.

Insoluble in water, soluble in alcohol and oils. B.P. 214° C.

Oily, but slightly pungent-fruity, herbaceous odor of moderate to poor tenacity. Less winey than Methylnonylketone (a naturally occurring isomer), and not quite as Orange-like. Greener and fruitier.

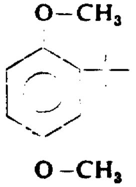
This ketone, rarely offered commercially, has been suggested for use in perfume compositions. However, after so much discussion about the possible hazards of using certain ketones (including the named isomer) in perfumes for cosmetic preparations, chances are that this ketone has little or no future in perfumery.

Prod.: from Valeric and Heptanoic acids by heating of the mixture over Thorium oxide to about 450° C.

86-27; 159-413;

## 468: tertiary-BUTYLHYDROQUINONE DIMETHYLETHER

*1,4*-Dimethoxy-*2-tertiary*-butylbenzene.



$C_{12}H_{18}O_2 = 194.28$

White needlelike crystals.

Almost insoluble in cold water, slightly soluble in hot water, soluble in alcohol and oils.

Warm, mossy-nutlike, root-like odor of excellent tenacity. The sweetness has some similarity to that of Musk Ambrette and Vetiver, while the earthy notes resemble Walnut and Oakmoss.

This material finds some use in perfume compositions as a modifier/fixative in Chypre, Ambre, "Oriental" types, etc.

It blends well with Coumarin, Clove bud oil, Oakmoss, Vetiver, Ionones, Amylsalicylate, Lavender, etc.

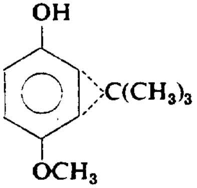
The title Diphenolether is rarely offered under its proper chemical name, but it enters many bases and specialties as a minor component. In view of the scarcity of Oakmoss-type perfume chemicals, this material should have some chances of becoming commonly used.

Prod.: from Hydroquinone and *iso*-Butylene, followed by complete Methylation of the Diphenol with Dimethylsulfate in weak aqueous alkali.

See also monographs: *3-tertiary*-Butyl-*4*-methoxybenzaldehyde, and:
*para-tertiary*-Butylresorcinol dimethylether.

## 469: BUTYL HYDROXY ANISOLE

Tenox BHA (Eastman-Tenneco Chem. Co.).
Embanox.
*1*-Hydroxy-*2-and-3-tertiary*-butyl-*4*-methoxybenzene.
Hydroquinone monomethylether, butylated.



$C_{11}H_{16}O_2$ = 180.25

Colorless (white) crystals. Insoluble in water, soluble in alcohol, soluble at 0.05 % to 0.20 % in most oils. Very faint phenolic type odor.

Used as an Antioxidant in foods, usually in combination with Propyl gallate and Citric acid for synergistic effect in Propylene glycol solution. Combinations with BHT (Butyl hydroxy toluene) are also used.

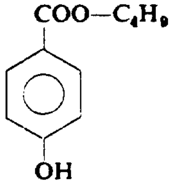
Prod. from *iso*-Butylene and *para*-Methoxyphenol.

Permitted for use in foods at limited level of concentration. (U.S.A.). (Limit: 0.5 % of the volatile portion of the flavorbase).

100-178; (Eastman/Tenneco data sheet).

## 470: BUTYL-para-HYDROXYBENZOATE

"Butyl paraben".
Butyl parasept.
Butoben.
Tegosept B.
Butyl chemosept.



$C_{11}H_{14}O_3$ = 194.23

White crystals or crystalline powder. Very faint odor. M.P. 69° C. Almost insoluble in water, soluble in alcohol. Slightly soluble in oils.

Classified as a preservative with a fungistatic effect 10 to 15 times higher than that of Benzoic acid.

Used as a preservative in cosmetic preparations at the concentration of 0.1 percent or less. Even at 0.05 % it may influence the effect of a given perfume to a certain degree, partly because it can be present at a concentration of 10 to 25 percent of the perfume itself thus becoming a significant factor in the fragrance performance. In general however, it will not seriously alter the fragrance.

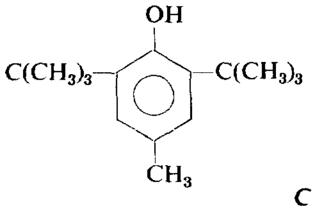
Prod. from Potassium salicylate via *para*-Hydroxybenzoic acid to the ester.

G.R.A.S. (June 1967).

100-181;

## 471: BUTYL HYDROXYTOLUENE

Tenox BHT. (Tenneco/Eastman).
Sustane. (U.O.P.).
D.B.P.C. (Koppers Co., Inc.).
2,6-Di-*tertiary*-butyl-*para*-cresol.
Ionol (Shell).
Improvol.
Vianol.
Dalpac FG (Hercules Powder Co.).



$C_{15}H_{24}O = 220.36$

Colorless crystals. Very faint musty, occasionally cresylic type odor. M.P. 70° C.
B.P. 265° C.

Insoluble in water, soluble in alcohol and Propylene glycol. Soluble in most oils and essential oils at 0.05 to 1.0%.

Used as an Antioxidant in foods, chemicals, perfume materials (natural and synthetic), etc., often in combination with Butyl hydroxy anisole (BHA) and Propyl gallate, Citric acid, etc. in Propylene glycol solution.

Will rarely influence the odor of the raw material or the composition in which it is incorporated at normal recommended use level.

Permitted for use in foods at limited level of concentration*) in the U.S.A.

Prod. from *para*-Cresol and *iso*-Butylene.

100-179; Tenneco data sheet.
*) see detailed information in: 162-586;

## 472: BUTYLIDENE ACETONE

*3*-Hepten-*2*-one.
Methyl pentenyl ketone.
Hepten-*3*-one-*2*.

$CH_3—CH_2—CH_2—CH{=}CH—CO—CH_3$

$C_7H_{12}O = 112.17$

Colorless oily liquid. B.P. 162° C.

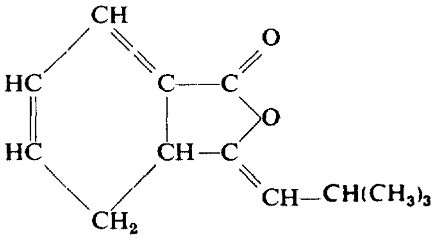
Almost insoluble in water, soluble in alcohol and oils.

This ketone, an isomer of the next lower homologue of Methylheptenone, has been suggested for use in perfumes, but it does not seem to be commercially available from the normal suppliers of perfume chemicals.

Its powerful, grassy-green, pungent odor and rather poor tenacity could place it among materials for perfuming of household products, detergents, etc., but since low-grade Methylheptenone is plentifully available from the Ionone manufacturers, there is probably not much interest in the title material.

Prod.: by condensation of Butyraldehyde with Acetone.

## 473: 3-iso-BUTYLIDENE-3a,4-DIHYDRO PHTHALIDE



$C_{12}H_{14}O_2 = 190.24$

Pale yellowish oily liquid. Slightly soluble in water. Soluble in alcohol and oils.
B.P. 278 C. Sp.Gr. 1.09.

Very powerful odor reminiscent of Celery juice and Celery seed, warm, penetrating and tenacious (soup-like dry-out odor).

Suggested for use in flavor compositions for "reconstitution" of soup flavor, meat flavor, etc. and for spice blends, condiments, dressings and appetizers.

NOT included in the G.R.A.S. list of the U.S. Federal Register, but it is most conceivable that this chemical, being a key constituent of natural vegetables, will be accepted for use as a synthetic material.

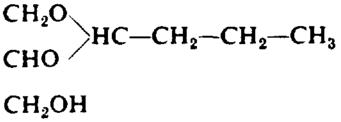
Prod. from Phthalic anhydride and *iso*-Valeric acid, using anhydrous Sodium acetate under heating to 180° C.

Litt.: Journal of Organic Chemistry 28, 985 (1963) (Gold and Wilson, authors). U.S. Agricultural Research Service. October 1962.

90-626;

## 474: 1,2-BUTYLIDENE DIOXYPROPANOL

Glycerol-*1*,*2*-butylacetal (cyclic).
*2*-Propyl-*4*-hydroxymethyl-*1*,*3*-dioxolane.



$C_7H_{14}O_3 = 146.19$

Straw-colored or yellowish viscous liquid. Somewhat soluble in water, soluble in alcohol and oils.

Warm-caramellic odor with a winey type of undertone.

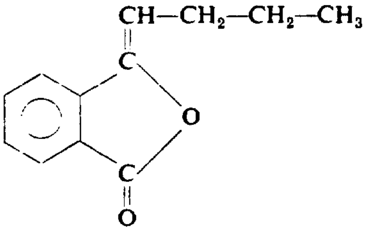
Suggested for use in flavor composition. Several other acetals of Glycerin and acetal mixtures are used in flavor creation.

Prod. from Glycerin and Butyraldehyde.

Litt.: A. Dupire: Comptes rendus 214 (359-360) 1942.

## 475: 3-n-BUTYLIDENE PHTHALIDE

Ligusticum lactone.



$C_{12}H_{12}O_2 = 188.23$

Yellowish oily liquid. B.P. 288° C.
Sp.Gr. 1.10.

Very slightly soluble in water, soluble in alcohol and oils. Heavy, warm-herbaceous. "soupy" odor, suggestive of Lovage root and somewhat reminiscent of Celery, but heavier.

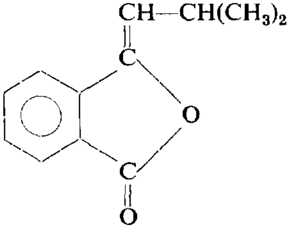
Suggested for use in flavor compositions for meat flavor blends, soup flavors, seasonings, dressings, sauces, etc.

NOT included in the U.S. Federal Register G.R.A.S.-list, but is most likely to become accepted since it is a known component of common vegetables.

Prod. from Sodium valerate, Valeric anhydride and Phthalic anhydride.

90-628;
Journal of Organic Chemistry 28, 985 (1963).
U.S. Agricultural Research Service, Oct. 1962.

## 476: 3-iso-BUTYLIDENE PHTHALIDE



$C_{12}H_{12}O_2$ = 188.23

Yellowish oily liquid with greenish fluorescence, or sometimes bluish-green fluorescence in dilution.

Powerful Celery-like, warm-herbaceous, spicy odor of great tenacity.

Celery-like taste, pleasant in dilutions below 0.1 ppm, but somewhat pungent-bitter at higher levels. Not nearly as "Lovage"like as the *3-n*-Butylidene phthalide (previous monograph), but more Celery-like.

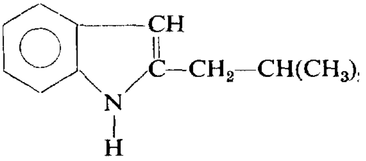
Suggested for use in soup flavor blends, meat flavors, dressings, appetizers, etc., but has not found much enthousiasm. Other derivatives seem more versatile in use.

Could be produced synthetically from Phthalic anhydride, Sodium *iso*-valerate and *iso*-Valeric anhydride, but this chemical is, to the author's knowledge, not available commercially as a synthetic.

Journal of Organic Chemistry 28, 985 (1963)
90-629;

## 477: alpha-iso-BUTYL INDOLE

*2-iso*-Butyl indole.
Presumably part of – or chief component of several well-known "Indole"-specialties.



$C_{12}H_{15}N$ = 173.26

White crystals. M.P. 60° C. B.P. 256° C.

Soluble in alcohol and oils, almost insoluble in water.

Powerful, diffusive odor, less pungent than that of Indole, overall milder and more floral, particularly in proper dilution.

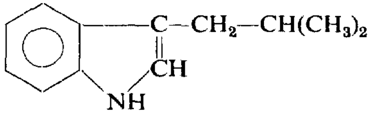
Used in perfume compositions as a modifier for Indole, or by itself as a delicately floral, very powerful, diffusive ingredient in floral bases, floral fragrance types, etc. It appears in the topnote as well as in the dryout of the fragrance in which it is incorporated, when applied at correct concentration. For Jasmin bases, concentrations in excess of one percent may be used, but other floral types can benefit from much smaller percentages.

Prod. from Indole.

4-70; 86-63;

## 478: beta-iso-BUTYL INDOLE

*3-iso*-Butyl indole.
(*iso*-Propyl skatole).



$C_{12}H_{15}N$ = 173.26

White crystals. Practically insoluble in water, soluble in alcohol and oils. B.P. 270° C.

Powerful diffusive odor reminiscent of Skatole more than of Indole, but considerably milder, not as offensive as Skatole. There is a marked difference in odor between this chemical and the *alpha*-isomer (previous monograph).

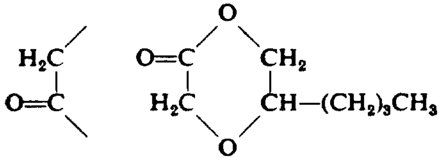
Suggested for use in perfume compositions, but does not seem to offer distinct advantages over Skatole-Indole mixtures.

Prod. from Indole.

86-73; 31-193; 5-312;

## **479: 2-BUTYL-5-(or 6-)-KETO-1,4-DIOXAN**

Commercial product may be a mixture of the isomers:



6-Keto- 5-Keto-

$C_8H_{12}O_3 = 156.18$

Colorless liquid. Poorly soluble in water, soluble in alcohol.

Powerful, fruity odor with winey-caramellic undertone.

Sweet-fruity and somewhat pungent-ethereal taste, unless diluted below 30 ppm.

This keto-ether is used in flavor compositions in mere traces to assist fruity notes, lend power and sweetness. It is used particularly for flavors intended for baked goods, candy, etc. and occasionally in Ice-cream flavors.

Concentration will normally be about 2 to 8 ppm. in the finished product.

F.E.M.A. No.2204.

Prod.: from Butyl ethylene oxide.

see also: Amyl ketodioxan.

## **480:** iso-**BUTYLKETONE**

*2*,*6*-Dimethyl heptan-*4*-one.
Di-*iso*-butyl ketone.
*iso*-Nonanone.
*iso*-Valerone.

$(CH_3)_2CH—CH_2—CO—CH_2—CH(CH_3)_2$

$C_9H_{18}O = 142.24$

Colorless oily liquid. Sp.Gr. 0.81.
B.P. 168° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, diffusive, fruity and sweet odor, often with a "butyric" undertone, poor tenacity.

Sweet Pineapple-Banana-like fruity taste, but with a somewhat harsh chemical note.

Occasionally used in perfumery for industrial masking odors where diffusive, volatile materials are desirable.

Prod. (several methods) e. g. by hydrogenation of Di-*iso*-butyl-carbinol.

26-486; 66-517; B-I-710; 36-1143;

## **481:** n-**BUTYL LACTATE**

Butyl-*alpha*-hydroxypropionate.

$CH_3(CH_2)_3—OOC—CHOH—CH_3$

$C_7H_{14}O_3 = 146.19$

Colorless liquid. B.P. 200° C. Sp.Gr. 0.97.

Slightly soluble in water, miscible with alcohol and oils.

Faint buttery-fruity odor with caramellic undertone.

Sweet buttery-caramellic taste, but very weak.

Used in flavor compositions for imitation Butter, various fruit flavors, Caramel, Treacle, Butterscotch, Rum, etc.

Concentration is usually traces (a few ppm) in the finished product.

Prod.: see Industr. Engin. Chem., 1940, vol. 32, page 692.

G.R.A.S. F.E.M.A. No.2205.

26-444; 66-786;

## 482: n-BUTYL LAURATE

*n*-Butyl dodecanoate.
*n*-Butyl dodecylate.

$CH_3(CH_2)_2CH_2—OOC—(CH_2)_{10}—CH_3$

$C_{16}H_{32}O_2 = 256.43$

Colorless oily liquid. Sp.Gr. 0.865.

Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Mild oily odor, but very pure grades of this chemical are virtually odorless. However, a distinct organoleptic effect is perceptible when this chemical is blended with lower boiling materials.

Used in flavor compositions, mainly for Apricot, Peach (for fatty-oily notes) and Brandy and Cognac (imitation of the fatty notes).

In various types of fruit flavors, accompanied by low-boiling esters. Concentration in the finished product is usually about 40 ppm.

Prod. by direct esterification of *n*-Butanol with Dodecanoic acid. When technical grade Lauric acid is used, the ester will carry Butyl esters of Decanoic (lower) and higher fatty acids.

G.R.A.S. F.E.M.A. No.2206.

86-27; 103-112;

## 483: n-BUTYL LEVULINATE

*n*-Butyl laevulinate.
*gamma*-Ketovaleric acid, *n*-butylester.
*n*-Butyl acetopropionate.

$CH_3(CH_2)_3OOC—CH_2—CH_2—CO—CH_3$

$C_9H_{16}O_3 = 172.23$

Colorless or pale straw-colored liquid. Slightly soluble in water, soluble in alcohol and oils. B.P. 238° C. Sp.Gr. 0.97.

Sweet and slightly pungent-caramellic odor with fruity undertones. Overall warm and almost herbaceous with some similarity to Valerolactone.

Mild, sweet, caramellic-herbaceous taste.

Used in flavor compositions for imitation Butter, Rum, and in various fruit flavors, "Tutti-frutti", etc.

Concentration is usually mere traces (a few ppm.) in the finished product.

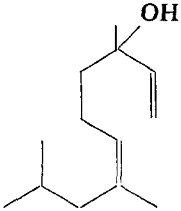
Prod. by direct esterification of *n*-Butyl alcohol with Levulinic acid.

G.R.A.S. F.E.M.A. No.2207.

26-444; B-III-207 (dritter Ergänzungsband).

## 484: iso-BUTYL LINALOOL

*3,7,9*-Trimethyl-*1,6*-decadien-*3*-ol.



$C_{13}H_{24}O = 196.34$

Colorless, slightly oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Sweet-fruity, somewhat floral and rich-woody odor. This odor complex resembles to some extent that of several of the popular "carbinols". The tenacity is moderate to good.

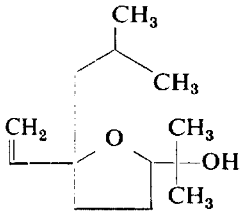
This alcohol was marketed shortly after synthetic Linalool became popular, and new derivatives were developed in search of more lasting and floral materials. The title material is not typically floral, it has a slightly dry-green note which is easily altered into a woody note in compositions. This type of odor can be used in Muguet, Rose, Bergamot and certain light, green-floral and woody-floral fragrances. So far, the material has definitely failed to catch any strong interest among the perfumers, probably due to lack of versatility and to the relatively high cost of this material.

Prod.: from Methyl-*iso*-butylketone and Acetylene in the synthesis used for production of Linalool.

sample: Hoffmann-laRoche, Inc.

## 485: iso-BUTYL LINALOOL OXIDE

2-Hydroxy-*iso*-propyl-5-*iso*-butyl-5-vinyl tetrahydrofuran.



$C_{13}H_{24}O_2 = 212.34$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Vinous-fruity and floral odor with a distinct Melon-Apple-like note. Good tenacity and considerable diffusive power.

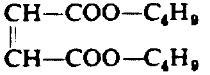
Dilutions at less than 20 ppm show a pleasant Apple-Banana-like taste, but higher concentrations seem to lack sweetness.

This oxide, very rarely offered commercially, but occasionally appearing from various research laboratories, has been suggested for use in perfume compositions. It could lend intetesting notes to fresh floral and floral-fruity fragrance types, and it blends very well with the sweet-green or mild-green, floral top-note chemicals.

Prod. from *iso*-Butyl linalool by oxidation with special oxidizing agents (e. g. Benzoyl peroxide).

## 486: BUTYL MALEATE

Di-*n*-butyl maleate.
Di-*n*-butyl butene dioate.
Di-*n*-butyl toxilate.



$$\begin{array}{l} CH-COO-C_4H_9 \\ \| \\ CH-COO-C_4H_9 \end{array}$$

$C_{12}H_{20}O_4 = 228.29$

Colorless liquid. B.P. 258° C. (decomp.).

Practically insoluble in water, soluble in alcohol and oils.

Faint, winey odor of good tenacity, but with a chemical undertone.

Mild, slightly bitter taste.

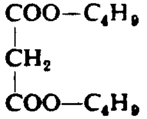
Apart from very occasional application as a modifier-blender in certain flavor compositions (NOT permitted in the U.S.A.), the author is not aware of any regular use of this ester in perfumes or flavors.

Prod. by direct esterification of *n*-Butanol with Maleic acid.

26-486;

## 487: BUTYL MALONATE

Di-*n*-butyl malonate.
Di-*n*-butyl propandioate.
Di-*n*-butyl methanedicarboxylate.



$$\begin{array}{l} COO-C_4H_9 \\ | \\ CH_2 \\ | \\ COO-C_4H_9 \end{array}$$

$C_{11}H_{20}O_4 = 216.28$

Colorless, slightly oily liquid. B.P. 252° C. Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Mild, ethereal-winey odor with a fruity undertone, yet somewhat hard or chemical.

Suggested for use in flavor compositions as a modifier for lower esters of Malonic acid, mainly in Apple, Wine, Gooseberry, Rum and

Plum. The ester is NOT listed specifically in the U.S.A. Federal Register's G.R.A.S.-list but may be used in certain countries in limited concentrations. Other Malonic esters are permitted, but very few Butyl esters are permitted. However, the Malonic acid itself has been questioned as to its absolute harmlessness.

Prod. from Cyanoacetic acid and *n*-Butanol in presence of Hydrochloric gas.

4-26; 26-486; 66-962; B-II-581;

## 488: n-BUTYL MERCAPTAN

Butanethiol-*1*.
*n*-Thiobutyl alcohol.

$C_4H_9-SH$

$C_4H_{10}S = 90.19$

Colorless mobile liquid. B.P. 98° C.
Sp.Gr. 0.834.

Slightly soluble in water, soluble in alcohol and oils.

Powerful, diffusive odor, reminiscent of Cabbage. Often described as Skunk-like, or just "sulfuraceous". If the reader is not familiar with the odor of a Skunk, any other odor description will be pretty far from proper. In extreme dilution, the odor becomes intensely sweet and finally "nondescript", but the threshold level of olfactory perception for this chemical is extremely low.

The taste is slightly bitter.

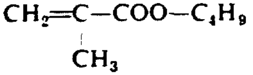
Has been suggested as a trace component for certain fragrance types, and – in rare cases – for flavor compositions for vegetable soup flavors. The author believes, however, that there is no regular use of this chemical in perfume or flavor creation.

Prod. from *n*-Butanol plus Hydrogen sulfide over catalyst.

4-194; 26-444; 66-347; 100-182; B-I-370;

## 489: n-BUTYL METHACRYLATE

*n*-Butyl-*alpha*-methylacrylate.
*n*-Butylpropen-*1*-carboxylate.



$$CH_2{=}\underset{\displaystyle CH_3}{\underset{|}{C}}-COO-C_4H_9$$

$C_8H_{14}O_2 = 142.20$

Colorless mobile liquid.

Almost insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Powerful, diffusive, gassy-ethereal, sweet-herbaceous odor with a warm-winey undertone and rather poor tenacity.

Sweet, slightly fruity and herbaceous taste.

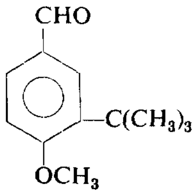
Suggested for use in artificial Chamomile, but has been replaced by the Angelate, which is more true-to-Nature and also more stable.

Produced by ester exchange reaction.

NOTE: Methacrylates in general are not welcome by the authorities for use in food, and they are mostly unstable, unsuitable for use in perfumes under the conditions prevailing in most cosmetic functional products.

## 490: 3-tertiary-BUTYL-4-METHOXY BENZALDEHYDE

*meta-tertiary*-Butyl anisaldehyde.



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid, solidifying in the cold.

Insoluble in water, soluble in alcohol and oils.

Powerful, woody-floral odor of considerable tenacity.

This aromatic aldehyde has been suggested for use in perfume compositions as a modifier for Anisaldehyde, Acetanisole, etc. However, its odor type is not immediately agreeable, it is rather harsh and it requires considerable skill and experience to incorporate the item in a floral or sweet-woody or sweet-herbaceous fragrance.

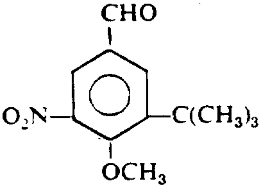
Since the material does not represent any exceptional or very pleasant odor type, there is probably not much future in the subject chemical.

Prod.: By oxidation of *meta*-Butylhydroquinone monomethylether.

4-133;

## 491: 3-tertiary-**BUTYL**-4-**METHOXY**-5-**NITROBENZALDEHYDE**

*3-tertiary*-Butyl-5-nitroanisic aldehyde.



$C_{12}H_{15}NO_4 = 237.26$

Pale yellowish crystals, soluble in alcohol and oils, almost insoluble in water.

Sweet-musky, rather harsh-herbaceous odor.

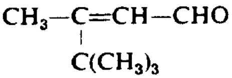
Has been suggested for use in perfumes, but has long since been bypassed by superior, more stable, non-discoloring and more distinct smelling Nitro- or non-Nitro-musks.

Note: A number of higher homologues (-ETHOXY-, PROPOXY-, and other Butyl-alkoxy nitrobenzaldehydes) have been mentioned in perfumery literature as possible candidates for use in perfume compositions. The author believes that all of these materials can be considered obsolete.

48-294; see also: 156-291;

## 492: beta-tertiary-**BUTYL**-beta-**METHYLACROLEIN**

*beta-tertiary*-Butyl crotonaldehyde.
Methyl-*iso*-amylidene acetaldehyde (incorrect name).



$CH_3-\underset{\displaystyle C(CH_3)_3}{C}=CH-CHO$

$C_8H_{14}O = 126.20$

Colorless or pale straw-colored liquid.

Powerful herbaceous, rather sweet odor, reminiscent of Clovercomplex, including the Coumarin-type of odor.

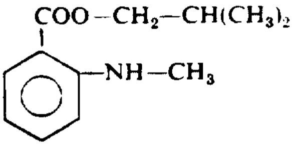
Has hardly any interest beyond the academic interest of studying chemicals with Coumarin-type of odor. There is no obvious similarity to the Coumarin (9 Carbon atoms, and no aldehyde group) or Octalactone (8 Carbon atoms and no aldehyde group), but the tertiary Butyl group as such has attracted much attention among those studying the possible relation between human olfactory perception and chemical structure.

Prod.: by condensation of Methyl-*iso*-butyl ketone and Acetaldehyde.

3-190; 4-214; 86-154;

## 493: iso-**BUTYL**-N-**METHYLANTHRANILATE**

*N*-Methylamino-*iso*-butylbenzoate.



$C_{12}H_{17}NO_2 = 207.28$

Pale straw-colored or almost colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet and floral-fruity odor of Petitgrain-Grapefruit type. Good tenacity and very attractive overall fragrance.

Sweet, fruity Grape- and Grapefruit-like taste in concentrations below 20 ppm. Many flavorists find that this ester produces more natural notes than any other Anthranilate.

This ester – although known for several decades – was almost never to be found in the price lists of the perfume chemical manufacturers. Only during the past 5 or 10 years, it has become better known and much more in demand. One reason may be that the technique of making Anthranilates has improved considerably, and there is now a distinct character to the individual esters, since they no longer carry a large amount of unreacted material.

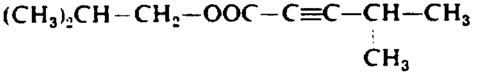
The title material gives very interesting effects in modern Colognes of the "old-fashioned" type, sometimes classified as "Continental" types or described by the name of some of the best known European Citrus colognes. It is also of value in Jasmin, Gardenia, Honeysuckle, Neroli, etc., and in Oriental fragrance types. It is pleasantly free from the "musty" note so often found in fragrances with too high concentration of Methylanthranilate (or Methyl-*N*-Methylanthranilate).

The ester could undoubtedly find extensive use in flavor compositions, if it would be included in the American G.R.A.S. list, which already contains several Anthranilates. It gives highly interesting effects in Citrus types, particularly Grapefruit, and it has a mellowing effect upon the American type of Grape flavor (which is predominantly a Methylanthranilate type, Concord Grape flavor). It could furthermore be used in "Tutti-frutti", in Plum, Apricot, Mango, etc.

Prod.: from *iso*-Butylanthranilate by Methylation or, more recently: from *N*-Methylisatoic anhydride plus *iso*-Butylalcohol by conventional esterification method.

## 494: iso-**BUTYL**-3-**METHYL**-n-**BUT**-1-**IN CARBONATE**

*iso*-Butyl-*iso*-hexynoate.



$$(CH_3)_2CH-CH_2-OOC-C\equiv C-\underset{\displaystyle CH_3}{CH}-CH_3$$

$$C_{10}H_{16}O_2 = 168.24$$

Colorless oily liquid. B.P. 200° C. Insoluble in water, almost insoluble in Propylene glycol, soluble in alcohol and oils.

Powerful, penetrating green "foliage" odor, between Violet leaf and Cucumber, but rather pungent-gassy in its approach, not as pleasant as the higher esters.

Suggested for use in perfumes as a modifier for Methyl heptin carbonate and other esters of acetylenic acids.

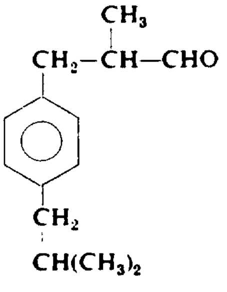
This particular ester has little to offer of interest to the perfumer, and it is most likely to disappear entirely in the vast number of unused research chemicals.

Prod. from *iso*-Valeraldehyde plus *3*-Methyl-*n*-but-*1*-yne.

5-245;

## 495: para-iso-**BUTYL**-alpha-**METHYL HYDROCINNAMIC ALDEHYDE**

"Rhodial" (Rhodia, Inc.).
"Homocyclamen aldehyde".
*alpha*-Methyl-*para*-*iso*-butyl hydrocinnamic aldehyde.
*2*-Methyl-*3*-*para*-*iso*-propylphenyl-*1*-propanal.



$$C_{14}H_{20}O = 204.31$$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Fresh, floral-green odor of moderate to good tenacity. The floral notes are predominantly Lily-Muguet-like, while the green notes resemble Watermelon rind. The material displays a distinctly balsamic undertone.

The title aldehyde, commercially available for some years, has some of the advantages of Cyclamen aldehyde, and some of those of Lilial (Bucinal), its *tertiary*-Butyl-isomer. It is undoubtedly more versatile than Cyclamen aldehyde, and the perfumer can enjoy using much higher concentrations of this aldehyde, without producing overly green-vegetable notes, etc.

The present cost (oct. 1968) is well below that of Lilial, and also more favorable than the price of Cyclamal. In brief, the material has most of the prerequisites for becoming a large-volume, commonly used fragrance chemical.

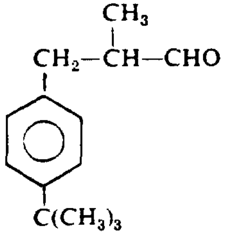
It blends very well with Lilac materials, Muguet (carbinols and rose-alcohols), Styrax and Methylionones, and with Amylcinnamic aldehyde. It is sufficiently stable in soap, and it seems to be more stable in storage than Cyclamen aldehyde.

Prod.: (many methods) e. g. from *para-iso*-Butylbenzaldehyde by condensation with Propionaldehyde under alkaline conditions, followed by selective hydrogenation of the unsaturated aldehyde to the title material.

(Literature: Rhodia, Inc.). 163-375; 156-151;

## 496: para-tertiary-**BUTYL**-alpha-**METHYL HYDROCINNAMIC ALDEHYDE**

*alpha*-Methyl-*para-tertiary*-butyl hydrocinnamic aldehyde.
*para-tertiary*-Butyl-*alpha*-methylhydrocinnamic aldehyde.
"Lilial" (Givaudan-Delawanna, U.S.A.).
"Bamca" (U.O.P. Chem. Co.).
Bucinal.
"Lily aldehyde" (Soda Aromatic Co., Japan).



$C_{14}H_{20}O = 204.31$

Almost colorless oily liquid. Sp.Gr. 0.96.
B.P. approximately 258° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, yet refreshing and intensely floral-green odor of considerable radiance, although at the same time quite tenacious. There are notes resembling Hydroxycitronellal, and other notes recalling Cyclamen aldehyde.

This aldehyde, developed later than Cyclamen aldehyde in search of interesting homologues, has found considerable interest in perfumery. It is widely used in soap perfumes and many cosmetic perfumes.

An excellent floralizer in itself, it also blends well with other floral materials, as well as with the musks and woody notes. It is far more versatile than Cyclamen aldehyde, or one can say that it is much more difficult to "overdose" Lilial than it is to overdose Cyclamal. Yet, Lilial gives floral effects at lower concentration than Hydroxycitronellal, a fact that almost compensates for the cost difference.

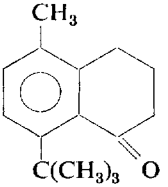
A conventional material in Lily, Lilac, Muguet, Orangeblossom, Magnolia, Sweet Pea, Frangipanni, it is also used in Chypres, Orientals, wood complexes and musky bases, as well as in modern fantasy soap perfumes, etc.

Lilial has, in the comparatively short time it has existed, grown to become one of the truly "large-volume" fragrance chemicals, with an estimated annual production of well in excess of 100 tons, counting Lilial, Bamca, Bucinal and other brands.

Prod.: by condensation of *para-tertiary*-Butylbenzaldehyde in Methanol with Propionic aldehyde under alkaline conditions, followed by hydrogenation.

106-217; 156-150;

## 497: 8-tertiary-**BUTYL**-5-**METHYL**-alpha-**TETRALONE**



$C_{15}H_{20}O = 216.33$

Several derivatives of Tetralone and Suberone have been suggested for use in perfumery because of their odor resemblance to Sandalwood. This chemical is one of the earlier ones, and it has lost its importance or interest since the appearance of Sandalwood-smelling chemicals developed from Guaiacol-research at lower cost and with closer resemblance to the Natural Sandalwood oil.

This chemical resembles in odor not only Sandalwood as such, but it carries an "incense"-like note that attracted the attention of the first observers.

The chemical is not regularly available from perfume chemical manufacturers.

Prod. from *3-tertiary*-Butyl-*2*-methyl-*gamma*-phenylbutyric acid plus anhydrous Aluminium chloride.

9-70; 86-125; see also: 30-252;
see also: *8-tertiary*-Butyl-*alpha*-benzosuberone.
*iso*-Bornyl methoxy cyclohexanol.
*7-tertiary*-Butyl-*alpha*-tetralone-*1*.

## 498: n-**BUTYL MYRISTATE**

*n*-Butyl tetradecanoate.

$C_4H_9—OOC(CH_2)_{12}CH_3$

$C_{18}H_{36}O_2 = 288.49$

Colorless oily liquid. Solidifies in the cold. Insoluble in water, soluble in alcohol and oils.

Mild, oily-fatty odor reminiscent of Castor oil.

Occasionally used in perfumery to introduce fatty, Orris-like notes or flower-wax notes in floral bases, artificial flower absolutes, etc.

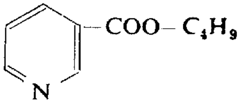
Occasionally used in flavor compositions for imitation Cognac and Nutmeg, again mainly for its peculiar fatty notes.

Prod. from *n*-Butanol and Myristic acid by direct esterification under azeotropic conditions.

103-112;

## 499: BUTYL NICOTINATE

*3*-Pyridinecarboxylic acid, *n*-Butylester.
*beta*-Pyridinecarboxylic acid, *n*-Butylester.



$C_{10}H_{13}NO_2 = 179.22$

Colorless oily liquid. B.P. 231° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Pungent-sweet, Mushroom-tobacco-like odor of moderate tenacity, but of great penetration.

Severals esters of Nicotinic acid are used sparingly in perfume compositions, although the chemical name seems to scare many perfumers from including any trace of it in their formulations.

The title ester finds use in heavy, exotic-floral as well as in woody-non-floral, "Oriental" type fragrances. It blends well with the Methylionones, with Jasmin base or flower absolute, Narcissus notes, Labdanum, Phenylacetic esters, Civet products, precious wood notes, etc.

This material is rarely offered commercially, but may be manufactured on a small scale by the individual users.

Prod.: from Nicotinic acid and *n*-Butanol by azeotropic type esterification.

163-329;

## 500: n-BUTYL OLEATE

$(C_4H_9)OOC—(CH_2)_7—CH{=}CH(CH_2)_7CH_3$

$C_{22}H_{42}O_2 = 338.68$

Pale yellowish oily liquid. Sp.Gr. 0.88. B.P. 232° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, oily, Linseed-oil-like odor, mild, but persistant.

Occasionally used in perfume formulation where this particular type of fatty note is desirable (flower absolute imitations, "petal"-notes, etc.) e. g. in artificial Jasmin absolute.

Prod. from *n*-Butanol and Oleic acid by heating to 100-150° C. with sulfuric acid as a catalyst.

26-444; 49-483; B-II-439, zweiter Ergzbd.

## 501: BUTYL OXALATE

Di-*n*-butyl oxalate.

$$\begin{array}{l} COO—C_4H_9 \\ COO—C_4H_9 \end{array}$$

$C_{10}H_{18}O_4 = 202.24$

Colorless liquid. Sp.Gr. 0.99. B.P. 248° C.

Insoluble in water, soluble in alcohol and oils.

Faint, nondescript odor between fruity and winey, rather pleasant but weak.

Has been suggested for use in perfumes as a solvent/blender, but does not seem to offer advantages over odorless or low-odor solvents conventionally used.

Prod. from *n*-Butanol and Oxalic acid by direct esterification.

4-26; 26-486; 66-956; B-II-540;

## 502: iso-BUTYL PELARGONATE

*iso*-Butyl nonanoate.
*iso*-Butyl nonylate.
NOTE: The *n*-Butyl ester is also used.

$(CH_3)_2CH—CH_2—OOC(CH_2)_7CH_3$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid. B.P. 260° C. Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Fresh, slightly oily-rosy, fruity odor reminiscent of Applepeel, Orange and Apricot, good tenacity.

Occasionally used in perfumes as a modifier for Amyl caprylate or similar fruity materials in lipstick fragrances or in bases where new fruity notes may be desirable.

This chemical blends well with rose-materials such as *iso*-Butyl phenylacetate, and with the simple Ionones, a conventional blend in lipstick fragrances.

Could find some use in flavor compositions, particularly in view of its good tenacity. It would act as a fixative on the lower boiling fruity chemicals and support the stability in flavors that become exposed to heat under preparation of the functional product (baked goods, candy, etc.).

Prod. by direct esterification of *iso*-Butanol with Nonoic acid under azeotropic conditions.

4-70; 35-514; 103-112; 140-143;

## 503: iso-BUTYL PENTADECYLATE

*iso*-Butyl pentadecanoate.
*iso*-Butyl tetradecane-*1*-carboxylate.

$(CH_3)_2CH—CH_2—OOC(CH_2)_{13}CH_3$

$C_{19}H_{38}O_2 = 266.51$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

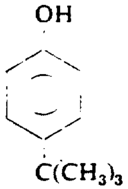
Almost odorless, but develops a flower-wax-like odor in blends with lower boiling fragrance materials.

It has therefore found occasional use in the making of artificial flower absolutes, Tuberose and Jasmin in particular. However, the Oleic esters seem superior for this purpose.

Prod. by direct esterification.

## 504: para-tertiary-BUTYL PHENOL

*1*-Hydroxy-*4*-*tertiary*-butylbenzene.
Butylphen.
(parent chemical in the manufacture of *para-tertiary*-Butyl cyclohexanol and -acetate).



$C_{10}H_{14}O = 150.22$

White needlelike crystals. M.P. 98° C.
B.P. 238° C.

Slightly soluble in water. Soluble in alcohol, oils and in aqueous alkali.

Powerful dry-leathery-phenolic odor, remotely reminiscent of the odor of certain Oakmoss products.

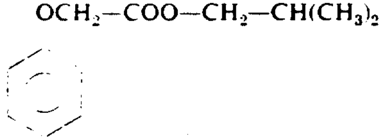
Suggested for use in perfume compositions to introduce Oakmoss-like or leather-like notes. It must be applied with great discretion since it tends to "grow" on the dryout notes, due to its great tenacity (low vapor pressure at room temperature).

This chemical suffers from the same drawbacks as the simple phenols: discoloration, non-stability in alkali media, etc. Yet, its application in detergent fragrances is already an established success.

Prod. from Phenol and *iso*-Butylene by heating with Zinc chloride, or directly from Phenol and *tertiary*-Butanol in alcoholic solution.

5-287; 26-444; 100-182; B-VI-524; 68-422;

## 505: iso-BUTYL PHENOXYACETATE



$OCH_2—COO—CH_2—CH(CH_3)_2$

$C_{12}H_{16}O_3 = 208.26$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

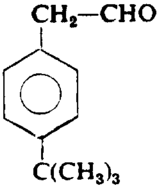
Sweet-herbaceous, Honey-like odor of considerable tenacity.

This ester has been used – and probably still finds some use – in Honey-bases for perfumery, the various "miel" types, etc.

That particular fragrance base is no longer fashionable, and only rarely used in today's perfumery. It has been used in conjunction with Allyl phenoxyacetate in such bases in the past.

Prod.: from *iso*-Butanol by esterification with Phenoxyacetic acid preferably under azeotropic conditions.

## **506:** para-tertiary-**BUTYL PHENYLACETALDEHYDE**



$C_{12}H_{16}O = 176.26$

Colorless oily or slightly liquid. B.P. 232° C.

Insoluble in water, soluble in alcohol and oils.

Pleasant, floral-green odor with soft-woody or green-bark-woody undertones. Fair to moderate tenacity.

This aldehyde, related to "Cortexal" and other popular specialties, has found a little use in perfumery, more in the floral fragrance types, not so much in the green topnote bases.

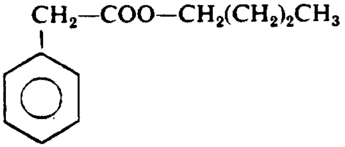
It blends well with Cyclamenaldehyde, Bucinal and other fresh-floral aldehydes, and with many Cinnamic derivatives.

Prod.: (numerous methods) e. g.: from *para-tertiary*-Butyl toluene via the substituted Benzaldehyde, glycidic ester, and saponification to the title aldehyde.

3-172; 86-126;

## **507:** n-**BUTYL PHENYLACETATE**

*n*-Butyl-*alpha*-toluate.



$C_{12}H_{16}O_2 = 192.26$

Colorless, slightly oily liquid. Almost insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.00. B.P. 258° C.

Somewhat hard or chemical Rose-Honey, slightly animal odor of good tenacity.

Sweet taste, honeylike with a slightly floral note.

Is very rarely used in perfumery, where the *iso*-Butylester is largely preferred (see next monograph).

Finds some use in flavor compositions (however, the author suspects that many materials labelled "Butyl phenylacetate" are actually *iso*-Butyl-): For imitation Butter, Caramel, Chocolate, Fruit (Tutti-frutti), Honey, Nut, Rose, etc.

Concentrations are usually about 12 to 15 ppm in the finished product.

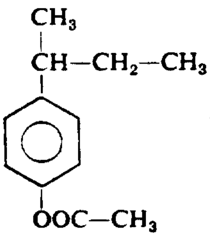
G.R.A.S. F.E.M.A. No.2209.

Prod. by direct esterification of *n*-Butanol with Phenylacetic acid under azeotropic conditions, or by direct reaction of Benzyl cyanide with *n*-Butanol under acid conditions.

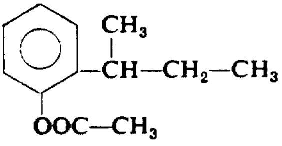
4-26; 26-444; 34-245;

## **508:** para-secondary-**BUTYL PHENYLACETATE**

This monograph includes the *ortho*-isomer.



*para-*



*ortho-*

$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquids. Insoluble in water, soluble in alcohol and oils.

Although these two materials have been offered separately, labelled individually as single and pure chemicals, there is reason to mention them under the same title. One was originally contaminated with the other, and the odor of the two materials had much in common.

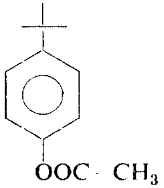
They are sweet, anisic-type odors of moderate tenacity. If they were made available at a cost competitive to common "anisic" odorants, it is possible that they could be used in quantity for technical perfumery, industrial fragrances, etc.

The anisic note is rather pungent, not harsh, but unnatural, yet powerful, and it is unlikely that the materials could be used in flavor compositions.

Prod.: by Acetylation of the corresponding phenols. These materials constitute results of research in connection with the manufacture of *para-tertiary*-Butyl cyclohexanyl acetate. (Agfa, Germany).

3-286; 4-26;

## 509: para-tertiary-**BUTYL PHENYLACETATE**



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

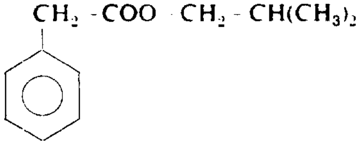
Musty-fruity odor of moderate tenacity and an overall unnatural character.

This ester, developed from research on the impurities in the popular *para-tertiary*-Butyl cyclohexyl acetate (the hydrogenated equivalent to the title material), has no importance in perfumery as such. It is mentioned in this work for the sake of completing the description of the materials related to the cyclohexyl-derivative which is normally marketed in the form of several reaction products, isomers, etc.

Prod.: by Acetylation of *para-tertiary*-Butyl phenol.

## 510: iso-**BUTYL PHENYLACETATE**

"Anther".
"Eglantine".
Phenysol.
"Iphaneine". (A.B.R.A.C.).
*iso*-Butyl-*alpha*-toluate.



$C_{12}H_{16}O_2 = 192.26$

Colorless slightly oily liquid. Sp.Gr. 0.98-0.99. B.P. 247 C.

Insoluble in water, almost insoluble in Propylene glycol, Glycerin and Mineral oil, soluble in alcohol and perfume or flavor materials.

Powerful and very diffusive leafy-rosy-musky odor with exceptional topnote effect. Distinctly fresher and more diffusive (not really volatile) than the *n*-Butylester. Slightly waxy notes (fresh, Narcisse-like) are typical of the pure product, while unpleasant or pronounced animal-honeylike notes dominate the poorer grades.

Finds extensive use in perfumery for fresh "petal" notes in Rose, Peony, Narcisse, Carnation, Sweet Pea, Freesia, Hyacinth, etc.

Useful in flavor compositions for imitation Butter, Caramel, Chocolate, Tutti-frutti, Honey, Nut, and – in mere traces – as a "lift" in Mint flavors for mouthwash, etc.

Concentrations are normally as low as 5 to 8 ppm in the finished product.

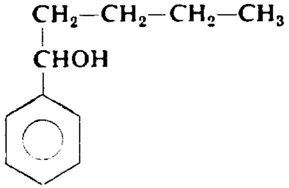
Produced by direct esterification of *iso*-Butanol with Phenylacetic acid under azeotropic conditions, or directly from Benzyl cyanide and *iso*-Butanol under acid conditions.

G.R.A.S. F.E.M.A. No.2210.
FCC - 1964 - 841;

4-71; 26-444; 34-245; 86-73; B-IX-435; 140-151;

## 511: n-BUTYL PHENYL CARBINOL

Phenyl butyl carbinol.
*alpha*-Butyl benzylalcohol.



$C_{11}H_{16}O = 164.25$

White solid lumps or crystalline powder.
M.P. 69° C. B.P. 285° C.

Insoluble in water, soluble in alcohol and oils.

Mild floral odor, slightly green, woody-barklike. One manufacturer classifies it as "Orris-like".

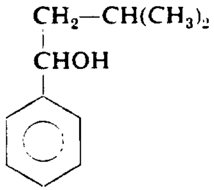
Useful as a fixative in Lilac or as a modifier-fixative for compositions where Linalool is present.

Prod. by reduction of Valerophenone with Sodium.

34-162;

## 512: iso-BUTYL PHENYL CARBINOL

Phenyl-*iso*-butyl carbinol.
*alpha-iso*-butyl benzylalcohol.



$C_{11}H_{16}O = 164.25$

White crystalline mass, M.P. 67° C.
B.P. 280° C.

Insoluble in water, soluble in alcohol and oils.

Mild floral odor, suggestive of Lindenblossom, a delicate combination of woody and floral with a discrete dryness.

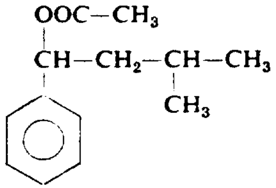
Occasionally used in perfume compositions as a modifier-fixative for Linalool or as a specific floral note in Muguet or Lilac, etc. However, this particular fragrance type is more pronounced and even more pleasant in *iso*-Butyl benzyl carbinol, the next higher homologue.

Prod. by reduction of *iso*-Valerophenone with Sodium.

86-115;

## 513: iso-BUTYL PHENYL CARBINYL ACETATE

Phenyl-*iso*-butylcarbinylacetate.
*2*-Methyl-*4*-phenylbutan-*4*-yl acetate.
*alpha-iso*-Butyl benzylacetate.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Fresh-woody, delicately fruity and green odor of moderate tenacity.

This "carbinol" acetate is not one of the more popular or common ones. It finds a little use in perfume compositions, mainly in Chypre or Fougère types, novel fantasy types, aldehydic-mossy types, etc. It is occasionally used in better soap perfumes, where its stability and solid undertones come to good effect.

The next higher homologue of the parent

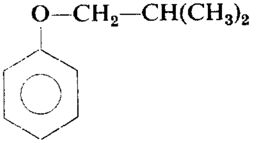
alcohol, *iso*-Butyl benzylcarbinol, finds more extensive use on account of its power and versatility.

Many carbinols and some of their esters perform very well in powder perfumes, and it is worth taking advantage of the relatively few materials which stand up so firmly and steadily with attractive fragrance in a powder.

Prod.: by direct esterification of the carbinol with Acetic acid under azeotropic conditions.

## 514: iso-BUTYL PHENYLETHER

Phenyl-*iso*-butylether.
*iso*-Butoxybenzene.
(commercially often called "Phenylbutylether").



$C_{10}H_{14}O = 150.22$

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Harsh-chemical odor, sweet, but with metallic-chemical background, remotely reminiscent of Anise. Cruder than Dihydro anethole (chemically related).

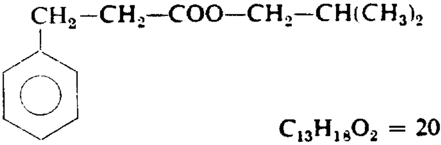
Could find some use in industrial masking odors on account of its power and fair tenacity. However, Anethole and *para*-Propyl anisole (Dihydro anethole) are commercially available in technical, lowcost grades and lend more immediate power to a composition.

Prod. from Sodium phenoxide with *iso*-Butylbromide in warm alcoholic solution – or: from *iso*-Butanol plus Phenol as vapors over catalyst at 420° C.

31-145; 31-147; 34-679; 86-114;

## 515: iso-BUTYL PHENYL PROPIONATE

*iso*-Butyl hydrocinnamate.



$C_{13}H_{18}O_2 = 206.29$

Colorless, slightly oily liquid.

Mild and sweet, floral-fruity odor with a faintly balsamic and animal undertone. Reminiscent of Strawberry, Rose and Lily.

Sweet-fruity, strawberry-like, rosy taste.

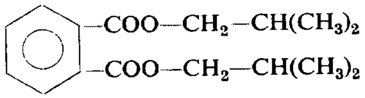
Finds a little use in perfumery as a modifying tool in fruity notes on floral backgrounds. For lipstick perfumes with Strawberry notes, or as a supporting topnote ingredient in Lily type fragrances.

The author is not aware of its use in flavor compositions, but this ester could probably find some use in Honey flavors, or it could constitute part of a sophisticated topnote in Peppermint flavors.

Prod. from *iso*-Butanol and Hydrocinnamic acid by direct esterification.

## 516: iso-BUTYL PHTHALATE

Di-*iso*-butyl phthalate.
(most common commercial product is: *n*-Butyl phthalate).



$C_{16}H_{22}O_4 = 278.37$

Colorless oily liquid. B.P. 334° C.
Sp.Gr. 1.04.

Almost insoluble in water, soluble in alcohol and oils.

Practically odorless when pure.

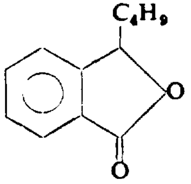
Has been used as a solvent-blender-diluent, but is now of little interest since Diethyl phthalate is available in an odorless grade and at very low cost.

Prod. from *iso*-Butanol and Phthalic anhydride or Phthalic acid.

See also: 100-182;

## 517: 3-n-BUTYL PHTHALIDE

(Previously called "Sedanolide").
(Sedanolide is now believed to be: Tetrahydro-*3-n*-butyl phthalide).



$C_{12}H_{14}O_2$ = 190.24

Almost colorless oily liquid. B.P. 280° C. Sp.Gr. 1.07.

Almost insoluble in water, soluble in alcohol and oils.

Warm-spicy, herbaceous odor, reminiscent of concentrated vegetable soup, suggestive of Celery and Lovage.

This interesting Lactone finds use in the composing of meat flavors, spice blends, etc. It is very powerful and comparatively stable to heat.

Being a naturally occuring component of several common vegetables or condiments, this chemical will most conceivably be accepted as a relatively harmless flavor material and should end up on the G.R.A.S. list.

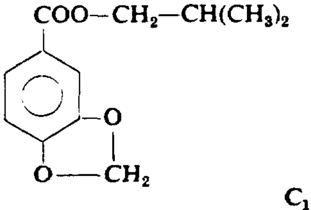
Sedanolide itself (see above) has mildly tranquillizing effect upon the human nervous system, but the doses required for this pharmacological effect are much higher than those suggested for flavor compositions, calculated upon the functional product.

Prod. from Phthalide via Bromation and reaction of the Phthalaldehydic acid with *n*-Butyl magnesium bromide.

65-692; 90-627;
Journal of the Chemical Society 1963, = 3, pages 1916-17-18-19;

## 518: iso-BUTYL PIPERONYLATE

*iso*-Butyl piperonilate.
Heliotropic acid, *iso*-butylester.



$C_{12}H_{14}O_4$ = 222.24

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Mild, balsamic-sweet and very tenacious odor, faintly floral, and warm.

This ester, rarely offered under its proper chemical name, finds limited use in perfume compositions, in which it can introduce very pleasant and fashionable "powdery" notes, supported by Anisylacetate, Cinnamylesters, Tolubalsam, high-grade Methylionones, Ambregris materials, etc.

It also blends well with Labdanum products, but it tends to reduce the – sometimes desirable – "dry-bitter" effect from certain types of refined Labdanum or Cistus products. In other words, the title material finds better use in distinctly sweet fragrance types.

Prod.: from Heliotropine via Piperonylic acid (by oxidation) followed by direct esterification under azeotropic conditions with *iso*-Butyl alcohol.

163-209;

## 519: n-BUTYL PROPIONATE

$C_4H_9{-}OOC{-}CH_2{-}CH_3$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 145° C.

Slightly soluble in water, miscible with alcohol and oils.

Ethereal-rumlike, rather heavy odor, yet volatile, diffusive.

Sweet rumlike, fruity taste, but not as fresh as the *iso*-Butylester.

Occasionally used in perfumes as a modifier in "vegetable-green" topnotes.

Used in flavor compositions for imitation Butter, Rum, Tutti-frutti, and various single fruit types.

Concentrations are usually about 30 ppm in the finished product.

Prod. by direct esterification of *n*-Butanol with Propionic acid (or Propionic anhydride) under azeotropic conditions. It is important that the esters of lower alifatic acids are free from water in order to make them free from acid during storage.

G.R.A.S. F.E.M.A. No.2211.

26-444; 77-184; 100-183; 103-106; B-II-241; 33-620; 140-137;

## 520: iso-BUTYL PROPIONATE

$(CH_3)_2CH{-}CH_2{-}OOC{-}CH_2{-}CH_3$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. B.P. 137° C.
Sp.Gr. 0.89.

Almost insoluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Diffusive, ethereal-fruity and sweet odor, reminiscent of Rum. Overall fresher and more rumlike than the *n*-Butylester.

Sweet taste in aqueous media, fresh and rumlike, finer than the *n*-Butylester.

Excellent base for imitation Rum flavors, but needs good fixation. Also very useful in imitation Butter, Peach, Strawberry, Tutti-frutti, and – in general – as a "lift" to numerous fruity types, to Caramel, Butterscotch, etc. Performs well in Icecream.

Concentrations are usually about 35 ppm in the finished product, but may be higher in Icecream and chewing gum.

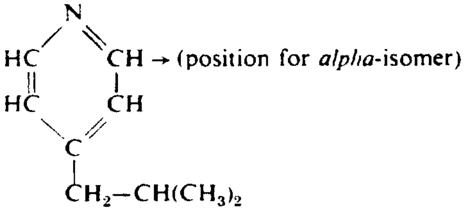
Prod. by direct esterification of *iso*-Butanol with Propionic acid (or Propionic anhydride) under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2212.

5-235; 26-444; 33-620; 100-573; 103-106; B-II-241;

## 521: iso-BUTYL PYRIDINE

Commercial samples have been mixtures of *alpha*- and *gamma*-isomers.
4-*iso*-Butyl pyridine.



*gamma*-isomer:
(most commonly mentioned)

$C_9H_{13}N = 135.21$

A number of alkyl-substituted Pyridines have been prepared since it was discovered that some of these have pleasant floral odors.

A pale yellowish oily liquid, almost colorless when freshly prepared. Practically insoluble in water, soluble in alcohol and oils.

Heavy-floral odor, somewhat reminiscent of Heliotrope. However, there is a marked difference in odor between the various samples submitted, and it is most conceivable that few, if any, are of truly high purity. Presence of traces of Pyridine base will destroy the floral odor picture, while considerable amounts of isomers can be present with little effect upon the odor.

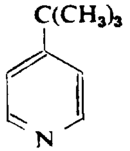
As long as this chemical is produced in such non-uniform batches, there is little chance of its acceptance by the perfumers.

Prod. from Pyridine with *iso*-Butyl bromide. The reaction product is a mixture of *alpha*- and *gamma*-isomers.

3-205; 30-266; 31-192;
(Reilly Tar & Chem. Co., Inc., pure isomers).

## 522: 4-tertiary-**BUTYL PYRIDINE**

*gamma-tertiary*-Butyl pyridine.



$C_8H_{13}N = 135.21$

Colorless or pale straw-colored liquid.

Insoluble in water, soluble in alcohol and oils.

Green-woody, slightly bark-like odor with striking resemblance to the odor of cured tobacco leaves (unflavored, but cured). In fact, the odor resembles that of a Cigarshop (without the smoke!)

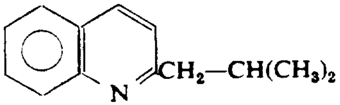
Many Alkyl-derivatives of Pyridines have been developed, and a number are mentioned in this work. Odor descriptions vary from one observer to the other, and it seems conceivable that the substituted Pyridines are often contaminated.

Undoubtedly, the purified Alkyl-pyridines represent a group of highly interesting perfume chemicals, and with the power they possess, one should be allowed to assume that the concentration needed in perfume compositions is so low that irritation hazards are eliminated or brought to a reasonable minimum. But it would still be wise to investigate such matter thoroughly prior to incorporating the materials in perfume for cosmetic purposes.

86-4;
(sample: Reilly Tar & Chemical Co., Inc.).

## 523: iso-**BUTYL QUINOLINE**-2

*alpha-iso*-Butyl quinoline.
(chief component of commercial *iso*-Butylquinoline).



$C_{13}H_{15}N = 185.27$

Colorless (when freshly distilled) oily liquid. Insoluble in water, soluble in alcohol and oils. Turns brownish if poorly stored (exposure to air and daylight).

B.P. approximately 255° C. Sp.Gr. 0.99.

Woody-earthy-mossy, slightly spicy odor, somewhat resembling Oakmoss (certain types of extract), Cardamom (with emphasis on the earthy notes) and, in extreme dilution, Ambre-like.

Trace amounts are frequently used in perfume compositions along with tenacious (high-boiling) fixatives such as Vetiver, Patchouli, macrocyclic musks, Oakmoss products, etc. If not properly fixed, the Quinoline odor will appear with undesirable strength in the dry-out of the fragrance. Effective concentrations may be less than 0.1 percent in the total perfume oil. The effect is more that of a general "lift" than actually an odor contribution, and the quinoline odor should not be part of the fragrance picture, but should appear with an undetectable note of radiation and strength.

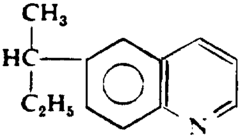
Occasionally used in Tobacco flavor compositions.

Prod. from *alpha-iso*-Butylamine and Acrolein.

28-559; 28-638; 77-213; 106-203; 156-319; 156-321;

## 524: iso-**BUTYL QUINOLINE**

*6-secondary*-Butyl quinoline.
(large component of *some* commercial *iso*-Butyl quinolines).



$C_{13}H_{15}N = 185.27$

Colorless, slightly oily liquid.

Insoluble in water, soluble in alcohol and oils.

B.P. approximately 252° C. Sp.Gr. 1.01.

Powerful earthy-tarry-mossy odor, at the same time sweet and dry, root-like.

Being different from the *2-n*-isomer with respect to odor, this chemical finds some use in perfumery, either because of direct odor preference on the part of some perfumers, or as a modifier for other isomers.

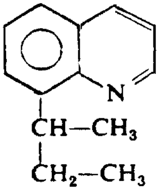
The pure chemical as such is not a commercially, regularly available item.

Prod. from *secondary*-Butyl aniline and Acrolein, followed by cyclization and oxidation.

4-70; 156-321;

## 525: 8-secondary-**BUTYL QUINOLINE**

*ortho-secondary*-Butyl quinoline.
(Often a minor component of commercial *iso*-Butyl quinoline).



$C_{13}H_{15}N = 185.27$

Colorless or pale straw-colored, slightly oily liquid. Insoluble in water, soluble in alcohol and oils.

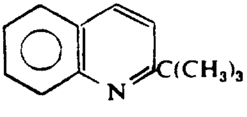
Powerful "Nicotine"-type odor, reminiscent of Tobacco-tars, "ashtray-odor", rather unpleasant. In extreme dilution almost floral and sweet.

Very rarely used in perfume bases to introduce special odor effects, mainly in floral absolute imitations, etc.

Generally considered an undesirable portion of the odor picture of commercial *iso*-Butylquinoline.

## 526: tertiary-**BUTYL QUINOLINE**

*2-tertiary*-Butyl quinoline.



$C_{13}H_{15}N = 185.27$

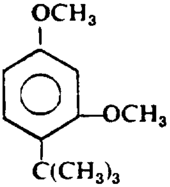
Almost colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Tobacco-like, also Nicotine-like, sweet-amine-type odor, not as unpleasant as that of *2-secondary*-Butylquinoline.

Of very little interest to the perfumer, beyond that of being a possible impurity in certain commercial lots of *iso*-Butylquinoline.

## 527: para-tertiary-BUTYL RESORCINOL DIMETHYLETHER

*1,3*-Dimethoxy-*4*-*tertiary*-butylbenzene.



$C_{12}H_{18}O_2 = 194.28$

Colorless oily liquid. Yellowish or brownish if improperly stored.

Insoluble in water, soluble in alcohol and oils.

Powerful earthy-spicy, warm and woody odor, remotely reminiscent of certain types of Oakmoss extract.

Has been suggested for use in artificial Oakmoss bases. Its spicy character falls very well in line with the Oakmoss odor and may be emphasized by addition of true spice materials to complete a fixative base of mossy-spicy type, at times very useful in men's fragrances as a fixative.

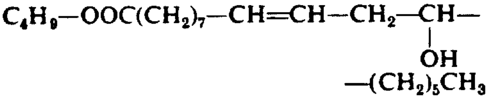
However, this chemical is extremely rare on the market, probably only manufactured for "captive use" by the manufacturing company.

Prod. from Resorcinol and *iso*-Butylene followed by Methylation of the phenol groups.

3-173; 4-195; 86-144;

## 528: BUTYL RICINOLEATE

*n*-Butyl-*12*-hydroxy-*9*-octadecanoate.



$C_4H_9{-}OOC(CH_2)_7{-}CH{=}CH{-}CH_2{-}\underset{OH}{\underset{|}{CH}}{-}(CH_2)_5CH_3$

$C_{22}H_{42}O_3 = 354.58$

Colorless oily liquid. Sp.Gr. 0.91.
B.P. 382° C.

Insoluble in water, soluble in alcohol and oils.

Very faint oily odor, strongly dependent upon purity of chemical.

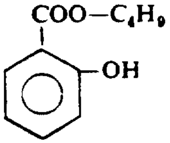
Suggested for use in perfume formulation to lend "oily" petal-like notes to certain floral bases.

Prod. from *n*-Butanol and Ricinoleic acid by heat.

4-26; 26-446; 100-183; B-III-388;

## 529: n-BUTYL SALICYLATE

Nefolia.
*n*-Butyl-*ortho*-hydroxybenzoate.



$C_{11}H_{14}O_3 = 194.23$

Colorless liquid, solidifying in the cold.
M.P. 6° C. Sp.Gr. 1.08. B.P. 268° C.

Somewhat rough-herbaceous-chemical odor, resembling Ethyl benzoate (but weaker) with a trace of Wintergreen note. Not as floral as *iso*-Butyl salicylate (next monograph). Not nearly as versatile as that ester, but quite powerful in compositions.

Used in perfume compositions as a modifier for higher esters of Salicylic acid. It produces a Fougere-like note with Coumarin and Lavandin – with or without Oakmoss – but not as attractive as the one obtainable with the Amylester. Blends well with the herbaceous oils, with Pine needle oils and related chemicals (Bornyl family), with Cedarwood products and it gives good fixative effect along with the simple Nitromusks in low-cost perfumes.

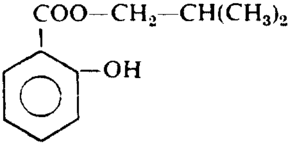
The hydroxyl group offers the conventional drawbacks of sensitivity to iron and alkali.

Prod. by direct esterification of *n*-Butanol with Salicylic acid under azeotropic conditions.

26-444; 33-733; 34-788; 103-113;

## 530: iso-**BUTYL SALICYLATE**

*iso*-Butyl-*ortho*-hydroxybenzoate.
"Isonefolia".



$C_{11}H_{14}O_3 = 194.23$

Colorless, slightly oily liquid. Sp.Gr. 1.07. B.P. 260° C.

Insoluble in water and Glycerine. Poorly soluble in Propylene glycol, soluble in mineral oil, alcohol and oils.

Overall sweet, but somewhat harsh-herbaceous-floral odor, generally described as resembling Clover and Orchid. However, the author finds that very few people – including perfumers – are familiar with the odor of (the very few) fragrant Orchids. The odor of this ester is less chemical in character than that of the *n*-Butylester, and upon extreme dilution, one can justly say that a fairly pleasant, green-floral odor appears.

Excellent blender with *iso*-Amylsalicylate or even substituting for this in Carnation types, Fougeres, Wallflower bases, etc. Blends well with *iso*-Bornyl acetate, Coumarin, Oakmoss. Lavandin and related oils, Ionones, Cedarwood products, Nitromusks, Peru balsam and many Citrus oils.

Traces of this ester are occasionally used in flavor compositions mainly for Rootbeer modifications, Fruit blends, etc.

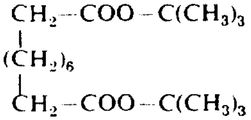
G.R.A.S. F.E.M.A. No.2213.

FCC-1964-843. Prod. by direct esterification of *iso*-Butanol with Salicylic acid under azeotropic conditions.

34-788; 95-188; 103-113; 106-204; 156-326;

## 531: tertiary-**BUTYL SEBACATE**

Di-*tertiary*-butyl decandioate.



$$\begin{array}{l} CH_2-COO-C(CH_3)_3 \\ | \\ (CH_2)_6 \\ | \\ CH_2-COO-C(CH_3)_3 \end{array}$$

$C_{18}H_{34}O_4 = 314.47$

Colorless oily liquid. Solidifies in the cold.

Insoluble in water, soluble in alcohol and oils.

Very faint, dry-musky odor, not as interesting as that of the *n*-Butyl sebacate.

Has at one time been suggested (and used) as a solvent for Nitromusks and a blender for same. However, it does not seem to offer any advantages over the newer solvents, and it does not contribute any highly interesting notes to the overall fragrance.

Prod. by direct esterification of *tertiary*-Butanol with Sebacic acid under azeotropic conditions.

## 532: BUTYL STEARATE

*n*-Butyl octadecanoate.

$C_4H_9—OOC—(CH_2)_{16}CH_3$

$C_{22}H_{44}O_2 = 340.59$

Colorless liquid. Sp.Gr. 0.86. B.P. 315° C.

Solidifies in the cold, M.P. 28° C.

Very slightly soluble in water, soluble in alcohol and oils.

Fatty, somewhat dry odor, practically odorless when pure. However, this ester does introduce interesting notes to fatty-fruity fragrances or flavors.

Occasionally used as a blender in Mimosa bases.

Occasionally used in flavor compositions for imitation Banana, Butter, Liquor, etc.

Concentrations may be as high as 350 ppm in the finished product, particularly when the ester is used as a fixative.

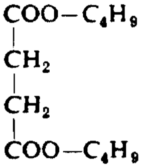
G.R.A.S. F.E.M.A. No.2214.

Prod. by direct esterification of *n*-Butanol with Stearic acid.

4-26; 26-446; 100-183; B-II-352, zweiter Ergzbd.

## 533: BUTYL SUCCINATE

Di-*n*-butyl succinate.
Tabutrex.



$$\begin{array}{l} COO-C_4H_9 \\ | \\ CH_2 \\ | \\ CH_2 \\ | \\ COO-C_4H_9 \end{array}$$

$C_{12}H_{22}O_4 = 230.31$

Colorless liquid, B.P. 275° C. Sp.Gr. 0.97.

Almost insoluble in water, soluble in alcohol and oils.

Virtually odorless, to some people displaying a faintly musky odor.

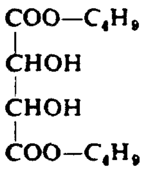
At one time used as a solvent for crystalline perfume materials. Now of little or no interest for such purpose. Has some insect repellant effect.

Prod. by direct esterification of *n*-Butanol with Succinic acid under azeotropic conditions.

4-26; 26-486; 100-343; B-II-551, zweiter Ergzbd.;

## 534: n-BUTYL TARTRATE

Di-*n*-butyl tartrate.



$$\begin{array}{l} COO—C_4H_9 \\ | \\ CHOH \\ | \\ CHOH \\ | \\ COO—C_4H_9 \end{array}$$

$C_{12}H_{22}O_6 = 262.31$

Colorless prismatic crystals or colorless liquid. Crystals melt at 23° C. Liquid Sp.Gr. 1.09. B.P. 300° C.

Almost insoluble in water, soluble in alcohol and oils.

At one time used as a solvent for crystalline perfume materials, but has no longer interest as such.

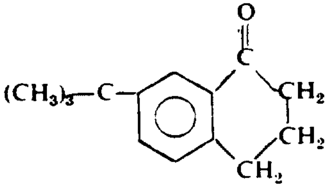
Practically odorless when pure.

Slightly bitter-astringent taste and mouthfeel.

Prod. by direct esterification of *n*-Butanol with Tartaric acid under azeotropic conditions.

4-26; 26-486; 86-27; B-III-518;

## **535:** 7-tertiary-**BUTYL**-alpha-**TETRALONE**-1



$C_{14}H_{18}O = 202.30$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Musky-woody, sweet and slightly camphoraceous odor, remotely reminiscent of Sandalwood odor.

Developed many years ago, before the chemically different "Sandela"-type of materials, this chemical was suggested for use as a Sandalwood odor. Its olfactory virtues, however, do not compete with the newer chemicals, and the Tetralone type will probably retire on the research shelf.

Prod. from *gamma(para-tertiary*-Butylphenyl)-butyryl chloride plus Benzene with Aluminium chloride condensing agent.

4-133; 4-284; 9-94; 30-251; 159-415;
See also: *8-tertiary*-Butyl-5-methyl-*alpha*-tetralone.
*8-tertiary*-Butyl-*alpha*-benzosuberone.
*iso*-Bornyl methoxy cyclohexanol.

## **536:** n-**BUTYL**-iso-**THIOCYANATE**

*n*-Butyl mustard oil.

$C_4H_9—N=C=S$

$C_5H_9NS = 115.20$

Colorless mobile liquid. B.P. 167° C.
Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils.

Lachrymator. Green-sharp, vegetable odor, diffusive and pungent-painful on human mucous membranes unless extremely diluted. Not as interesting as the *secondary*-Butylester.

Has been suggested as a modifier in condiment flavor blends and flavors for dressings and soups.

Prod. from *n*-Butylamine plus Carbon disulfide plus basic Lead acetate.

26-446; 66-946; 96-234; B-IV-158;

## **537:** iso-**BUTYL**-iso-**THIOCYANATE**

"*iso*-Butyl-*iso*-rhodanide".
*iso*-Butyl mustard oil.
(Sometimes called "Spoonwort oil, artificial", but this is truly the *secondary*-Butylester).
See next monograph.

$(CH_3)_2CH—CH_2—N=C=S$

$C_5H_9NS = 115.20$

Colorless or very pale yellowish mobile liquid.
B.P. 162° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

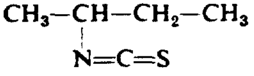
Lacrymator. Sharp, pungent, green-vegetable odor. In dilution it is less sweet than the *secondary*-Butylester, but more natural than the *n*-Butylester. Overall, this ester is of very little interest, but it has been suggested for use in flavor compositions for soups, dressings, sauces, spice blends, pickles, etc.

Prod. from *iso*-Butylamine plus Carbon disulfide plus basic Lead acetate.

26-446; 65-738; 95-206; B-IV-171;

## 538: secondary-**BUTYL**-iso-**THIOCYANATE**

*secondary*-Butyl-*iso*-rhodanide.
*secondary*-Butyl-*iso*-sulfocyanate.
"True Spoonwort oil".



$$\begin{array}{l} CH_3-CH-CH_2-CH_3 \\ \qquad\;\; | \\ \qquad\;\; N=C=S \end{array}$$

$C_5H_9NS = 115.20$

Colorless or pale yellowish mobile liquid.
B.P. 159° C. Sp.Gr. 0.94.

Insoluble in water, soluble in alcohol and oils.

Lachrymator. Sharp, but refreshing, vegetable odor type, slightly green. Pleasant in dilutions of less than 1 ppm.

The taste is inbetween that of Watercress and that of Cabbage (fresh).

Unstable in alcoholic solution. Unstable if exposed to acid under warm conditions.

Suggested for use in spice blends, soup flavors, meat sauce or pickle flavorings, etc.

Prod.:

1) from *secondary*-Butylamine plus Carbon disulfide plus basic Lead acetate, or
2) from Thiocarbonyl chloride plus *secondary*-Monobutylamine.

4-84; 26-446; 65-737; 66-946; 90-838; 95-506; B-IV-161; 140-177;

## 539: n-**BUTYL THIOGLYCOLATE**

*n*-Butyl mercapto acetate.

$C_4H_9-OOC-CH_2-SH$

$C_6H_{12}O_2S = 132.23$

Colorless oily liquid. Sp.Gr. 1.038.
B.P. 234° C.

Almost insoluble in water, soluble in alcohol and oils.

Faintly fruity, resembling Butylacetate-odor, but much weaker and not really Rum-like.

If it has ever been a manufacturer's intention that this ester should or could be used in perfumes or flavors, the author would recommend that it should not. This ester is unstable under acid conditions, even mild acid, and it will inevitably split off sufficiently of Hydrogen sulfide that a perfume or flavor composition eventually become ruined with this off-odor.

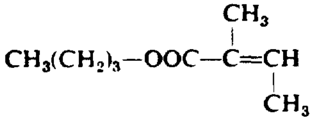
Needless to add that Hydrogen sulfide is extremely poisonous.

Prod. by direct esterification of *n*-Butanol with Thioglycolic acid under azeotropic conditions.

34-1245;

## 540: n-**BUTYL TIGLATE**

*n*-Butyl-*trans-alpha*-methylcrotonate.
*n*-Butyl-*2*-methyl-*2*-butenoate.
*n*-Butyl-*trans-beta*-dimethylacrylate.



$$CH_3(CH_2)_3-OOC-\overset{\displaystyle CH_3}{\overset{|}{C}}=\underset{\underset{\displaystyle CH_3}{|}}{CH}$$

$C_9H_{16}O_2 = 156.23$

Colorless liquid. B.P. 196° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, diffusive and almost gassy-ethereal odor, sweet and of moderate to poor tenacity.

This ester was developed for use in artificial essential oils, when Tiglic and Angelic acids became commercially available. However, the higher esters have become more popolar with their softer, less gassy odor and superior tenacity. Since the title ester has not been identified in Roman Chamomile oil, it is generally not preferred over the other esters for the purpose of making such artificial oil.

The material is probably almost obsolete today.

Prod.: by direct esterification of Tiglic acid with *n*-Butanol. Certain types of commercial Tiglic acid contain substantial amounts of Angelic acid which will be esterified along with the Tiglic acid.

The *iso*-Butylester of the isomer Angelic acid is included in the American G.R.A.S. list, and it is a naturally occurring ester.

## 541: n-BUTYL UNDECYLENATE

Butyl-*10*-undecenoate.

$C_4H_9{-}OOC(CH_2)_8CH{=}CH$

$C_{15}H_{28}O_2 = 240.39$

Almost colorless, oily liquid. Sp.Gr. 0.88. B.P. 252° C.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Buttery-fatty, winey odor, reminiscent of Brandy-residue. Very good tenacity.

Occasionally used in perfume compositions as a modifier for Costus oil and other Costus products, sometimes along with traces of Decalactone. It blends very well with the Ionones and most of the rosy smelling alcohols, etc.

Used in flavor compositions for imitation Butter, Apricot, Cognac, Brandy, Rum, Nut, etc.

Concentrations are usually about 50-70 ppm in the finished product.

Prod. by direct esterification of *n*-Butanol with Undecylenic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2216.

4-27; 35-854; 77-188; 86-27; (Baker Castor Oil Co., Inc.).

## 542: n-BUTYL VALERATE

*n*-Butyl-*n*-valerianate.
*n*-Butylpentanoate.

$C_4H_9{-}OOC(CH_2)_3CH_3$

$C_8H_{18}O_2 = 158.24$

Colorless mobile liquid. B.P. 186° C. Sp.Gr. 0.87.

Slightly soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Ethereal-fruity, somewhat choking odor, harsher than that of the *iso-iso*-ester.

Very sweet, fruity taste, suggestive of Apple and Strawberry.

Used in flavor compositions for imitation Apple, Butter, Chocolate, Fruit (and Tutti-frutti), Pineapple, Raspberry, Strawberry, etc.

Concentrations in the finished product are normally about 8-10 ppm.

Prod. by direct esterification of *n*-Butanol with *n*-Valeric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2217.

4-27; 5-238; 26-446; B-II-301; 85-38; 140-141;

## 543: iso-BUTYL VALERATE

*iso*-Butyl-*n*-pentanoate.

$(CH_3)_2CH—CH_2—OOC(CH_2)_3CH_3$

$C_9H_{18}O_2 = 158.24$

Colorless mobile liquid. B.P. 169° C. Sp.Gr. 0.86.

Almost insoluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Slightly fresher than the *n*-Butyl-*n*-valerate, however, this ester is the least interesting of the four isomers. It is merely included in this handbook for completion of the description of all Butylvalerates.

Prod. by direct esterification of *iso*-Butanol with *n*-Valeric acid under azeotropic conditions.

4-27; 5-238;

## 544: BUTYL-iso-VALERATE

*n*-Butyl-*iso*-pentanoate.
Butyl-*iso*-valerianate.

$C_4H_9—OOC—CH_2—CH(CH_3)_2$

$C_9H_{18}O_2 = 158.24$

Colorless mobile liquid. B.P. 167° C. Sp.Gr. 0.86.

Almost insoluble in water, soluble in Propylene glycol, miscible with alcohol and most oils.

Ethereal-fruity, Apple-like, somewhat pungent odor.

Sweet-fruity taste, reminiscent of Apple, Raspberry, with a winey note.

Occasionally used in flavor compositions, mainly in Chocolate flavors and fantasy fruit or Tutti-frutti, etc.

Concentrations are normally about 50 ppm in the finished product.

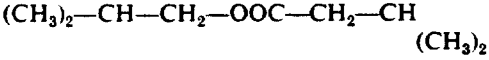
G.R.A.S. F.E.M.A. No.2218.

Prod. by direct esterification of *n*-Butanol with *iso*-Valeric acid under azeotropic conditions.

5-238; 26-446; 77-186; B-II-275, zweiter Ergzbd.;

## 545: iso-BUTYL-iso-VALERATE

*iso*-Butyl-*iso*-pentanoate.
(Sometimes referred to as "Butylvalerate").



$(CH_3)_2—CH—CH_2—OOC—CH_2—\underset{(CH_3)_2}{CH}$

$C_9H_{18}O_2 = 158.24$

Colorless mobile liquid. Sp.Gr. 0.872. B.P. 170° C.

Almost insoluble in water, soluble in Propylene glycol, miscible with alcohol and most oils.

Fruity-ethereal Apple-Raspberry-like odor. Fruitier than all other Butylvalerates. Probably the most interesting of the four isomers. Not as pungent-chemical as the other esters.

Occasionally used as a modifier in the fruity topnote of lipstickperfumes or other fruity cosmetic fragrances.

Widely used in flavor compositions for imitation Apple, Raspberry, Wine ("Champagne"), Strawberry, Tutti-frutti, etc.

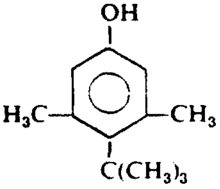
Although *iso*-Butyl-*iso*-butyrate is specifically mentioned in the G.R.A.S.-list of the Federal Register (U.S.A.), the *iso*-Butyl-*iso*-valerate is NOT mentioned. This could be an omission or an accidental confusion with the *n*-Butyl-*iso*-valerate, which is specifically mentioned. It has puzzled the flavor circles that the subject ester has been left out of the G.R.A.S. list.

Prod. by direct esterification of *iso*-Butanol with *iso*-Valeric acid under azeotropic conditions.

4-71; 5-238; 26-446; 33-732; 33-932; 103-112; B-II-312;

## 546: 4-tertiary-**BUTYL**-meta-3,5-**XYLENOL**

*para-tertiary*-Butyl-*meta-3,5*-dimethylphenol.



$C_{12}H_{18}O = 178.28$

White crystals. Very slightly soluble in water. Soluble in alcohol and oils.

Dry-tarry-leathery odor of considerable tenacity.

Occasionally used in Leather ("cuir") bases or Oakmoss compositions. Its odor is somewhat similar to that of *para-tertiary*-Butylphenol, but slightly sweeter.

Prod. from *iso*-Butylene and *meta-3,5*-Xylenol.

## 547: n-**BUTYRALDEHYDE**

*n*-Butanal.
Butyl aldehyde.
Butyric aldehyde.

$CH_3—CH_2—CH_2—CHO$

$C_4H_8O = 72.11$

Colorless liquid. B.P. 76° C. Sp.Gr. 0.82.

Soluble 6% in water, miscible with alcohol and oils.

Very diffusive, penetrating, pungent-irritating odor. Only in extreme dilution will truly fruity, Banana-like, green-fresh odor become perceptible.

Widely used in flavor compositions for imitation Banana, Butter, Caramel (Butterscotch), Brandy, Fruit (Tutti-frutti), Liquor, Nut, etc.

Concentration in the finished product may be as high as 4 to 5 ppm, but is in many cases much lower.

Very interesting and true-to-Nature effects can be obtained with combinations of this aldehyde and some unconventional flavor materials. For example, with Allyl-*iso*-thiocyanate in the proportion of 20 parts of the aldehyde to one part of the Allyl mustard oil, a typical "green-Banana" aroma when the mixture is diluted to 2-4 ppm, calculated upon the aldehyde.

NOTE: This aldehyde is flammable, and its vapors form explosive mixtures with air.

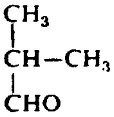
Prod.:
1) from *n*-Butanol vapors by catalytic oxidation.
2) from Crotonaldehyde by catalytic hydrogenation.

G.R.A.S. F.E.M.A. No.2219.

26-446; 36-1029; 66-477; 77-202; 100-183; B-I-662; 89-12; 140-157;

## 548: iso-**BUTYRALDEHYDE**

*iso*-Butyric aldehyde.
*iso*-Butyl aldehyde.
*2*-Methyl propanal.



$$\begin{array}{l} CH_3 \\ | \\ CH—CH_3 \\ | \\ CHO \end{array}$$

$C_4H_8O = 72.11$

Colorless mobile liquid. B.P. 64° C. Sp.Gr. 0.80.

11% soluble in water, miscible with alcohol and oils.

Extremely diffusive, penetrating odor, pungent and – undiluted – unpleasant, sour, repulsive. In extreme dilution it becomes almost pleasant, fruity, Banana-like, "overripe fruit-like". Overall more pleasant than the *n*-Butyraldehyde.

Widely used (in traces) in flavor compositions for imitation Banana, Berry, Butter, Caramel, Fruit, Liquor, Wine, Whisky and other flavors.

Concentration is conventionally lower than 5 ppm in the finished product.

See also comments under *n*-Butyraldehyde about mixtures with other flavor materials.

NOTE: This aldehyde is flammable, and its vapors form explosive mixtures with air.

Prod.:

1) from *iso*-Butanol vapors over catalyst at 250° C.
2) from Propylene plus Carbon Monoxide plus Hydrogen over catalyst at high pressure.

G.R.A.S. F.E.M.A. No.2220.

26-448; 66-477; 77-202; 100-573; B-I-671; 89-13; 140-157;

## 549: n-BUTYRIC ACID

Ethylacetic acid.
Butanoic acid.

$CH_3—CH_2—CH_2—COOH$

$C_4H_8O_2 = 88.11$

Colorless mobile liquid. B.P. 164° C. Sp.Gr. 0.96.

Solidifies in the cold, melts at minus 6° C.

Miscible with water, Propylene glycol, Glycerin, alcohol and oils.

Powerful, penetrating, diffusive sour odor, reminiscent of rancid butter. However, being water-soluble, the odor "airs out" easier from a room than one should expect, also it can be washed off the skin easily with water, leaving little or no odor if washing is performed immediately. Otherwise, the acid has a tendency to go "under the skin" and the sour odor will be perceptible for quite some times, resisting thorough washing or scrubbing.

Used in flavor compositions, primarily in Butter flavor. Also in imitation Cheese, Nut, Fruit, in Butterscotch and Caramel, Rum, etc.

Concentrations may be as high as 300 ppm (in imitation Butter) but will be much lower in most other functional products.

Prod. by controlled, selective fermentation of Carbohydrates. There are also several "chemical" synthetic ways, but the biochemical synthesis is an important one.

G.R.A.S. F.E.M.A. No.2221.

26-448; 90-61; 100-183; B-II-264; 77-184; 140-137;

## 550: iso-BUTYRIC ACID

*iso*-Propylformic acid.
*2*-Methylpropanoic acid.

$(CH_3)_2CH—COOH$

$C_4H_8O_2 = 88.11$

Colorless liquid. Sp.Gr. 0.95. B.P. 155° C.

Soluble 20% in water, miscible with Propylene glycol, alcohol and most perfume and flavor oils.

Powerful, diffusive sour (acid) odor, slightly less repulsive, and also less buttery than the *n*-Butyric acid. In extreme dilution the odor becomes almost pleasant, fruity.

The taste is, in proper dilution and with adequate sweetening, pleasant creamy-fruity, while buttery-cheesy notes are dominating in the absence of sweeteners. Sodium chloride enhances the buttery-cheesy flavor in that case.

Used extensively in imitation Butter, in Butterschotch and other Caramel types, in various fruit-flavor types, imitation Nut, Cheese, Vanilla, in Cream-soda flavor, Rum, Liquor, etc.

Concentrations are usually about 40 to 45 ppm in the finished product, except in chewing gum, where it may run as high as 450 ppm.

Prod. by oxidation of *iso*-Butanol.

G.R.A.S. F.E.M.A. No.2222.

NOTE: *iso*-Butyric acid has a pronounced ability to form azeotropes with a great number of solvents, aromatic chemicals, etc. This ability can be utilized in the preparation of esters with sensitive alcohols, such as Geraniol. The *iso*-Butyrate of that alcohol can be prepared by direct action of the acid or the anhydride using the acid as a carrier of water, thus preventing a breakdown of Geraniol. See Geranyl-*iso*-butyrate.

26-448; 77-184; 90-66; 100-573; B-II-288;

## 551: iso-BUTYRIC ANHYDRIDE

*iso*-Butyryl oxide.

$(CH_3)_2CH—CO—O—OC—CH(CH_3)_2$

$C_8H_{14}O_3 = 158.20$

Colorless liquid. Sp.Gr. 0.95. B.P. 182° C. Decomposes in presence of water or lower alcohols. Soluble in oils (but will react with many alcohols).

Sharp, irritating, acrid odor. Moisture in the air and in the human nostrils will produce *iso*-Butyric acid, which interferes with the true odor picture. However, the odor impression is distinctly different from that of the acid, and it shows the speed with which the human receptacles react and report the true odor.

Apart from this academic interest along the studies of human olfactory perception, the anhydride has very little interest as such to the flavorist.

It is a useful raw material to the perfume chemist in making esters of *iso*-Butyric acid.

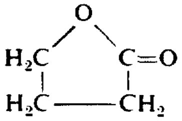
NOTE: Flammable liquid, but no hazard of explosive vapors under normal work temperatures.

Prod. from *iso*-Butyryl chloride and Sodium acetate, or: from *iso*-Butyryl chloride and Butyric acid with a catalyst.

26-448; B-II-292;

## 552: gamma-n-BUTYROLACTONE

*1,2*-Butanolide.
*1,4*-Butanolide.
*3*-(or 4-)-Hydroxybutyric acid, Lactone.



$C_4H_6O_2 = 86.09$

Colorless or very pale yellowish, oily liquid. Sp.Gr. 1.13. B.P. 204° C.

Miscible with water, Propylene glycol, alcohol and oils.

Faint, sweet-aromatic odor, rather nondescript.

Sweet, slightly caramellic taste, overall weak.

Has been suggested for use in flavor compositions, but it is most conceivable that its lack of power has prevented this Lactone from becoming a standard item on the flavorist's shelf.

The alkyl-substituted derivatives of this Lactone are, on the other hand, extremely interesting, and many of them have been used extensively for several decades in perfumes and flavors. (See Decanolide, Nonanolide, Undecanolide, etc.).

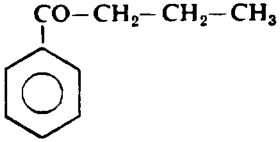
Prod. from:

1) Vinylacetic acid.
2) Glutaric acid.
3) Propion chlorohydrin via the Cyanhydrin.

30-254; 30-256; 30-268; 31-163; 66-799; 86-26; 100-184; 158-186;

## 553: BUTYROPHENONE

*n*-Propyl phenyl ketone.
Phenyl-*n*-propyl ketone.



$C_{10}H_{12}O = 148.21$

Colorless liquid. Solidifies in the cold, melts at 11° C. Sp.Gr. 0.99. B.P. 231° C.

Very slightly soluble in water, soluble in alcohol and oils.

Buttery-creamy, nutlike, somewhat herbaceous odor. There is a trace of resemblance to the Coumarins in this odor.

Sweet creamy-nutlike taste, but rather weak.

Finds little, or perhaps no use in perfumery.

Used occasionally in flavor compositions for imitation Walnut, Hazelnut, for Butterscotch, etc.

This chemical is NOT included in the American G.R.A.S. list.

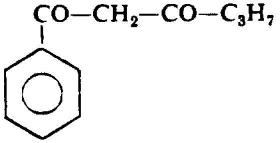
Prod. from Butyryl chloride plus Benzene with Aluminium chloride in a Friedel-Craft type synthesis.

Or, using Butyric anhydride instead of chloride.

4-27; 68-532; 86-28; 26-666; B-VII-313:

## 554: BUTYRYL ACETOPHENONE

*omega*-Butyryl acetophenone.
*1*-Phenylhexane-*1,3*-dione.



$C_{12}H_{14}O_2 = 190.24$

Yellowish oily liquid. B.P. 268° C.

Almost insoluble in water, soluble in alcohol, miscible with most oils.

Sweet and warm, woody-floral odor of Mimosa-Ylang type, carrying an oily, but not unpleasant overtone, resembling the topnote in Ylang-Ylang. Good tenacity.

This diketone has been suggested for use in perfume compositions, and it finds some use in the construction of artificial flower absolutes, bases and certain essential oils.

It is rarely offered under its proper chemical name, and almost never found in the price lists from manufacturers of perfume chemicals. However, it could find more extensive use, since it can be produced at relatively low cost, and it has considerable power in spite of its high boiling point.

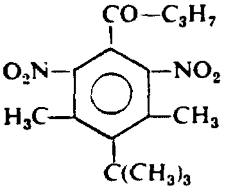
A limited use in fruity fragrances along with Ionones, Ethylmethylphenylglycidate, etc. shows a little of the versatility of this chemical. It performs very well in Strawberry (perfume) bases.

Prod.:

1) by condensation of Butylacetate with Acetophenone.
2) by condensation of Butyric anhydride with Acetophenone.

68-900; 86-28;

## 555: BUTYRYL DINITRO-tertiary-BUTYL-meta-XYLOL



$C_{16}H_{22}N_2O_5 = 322.37$

Pale yellowish crystalline powder.
M.P. 128° C.

Strong, sweet musky odor of considerable tenacity.

This material, closely related to "Musk Ketone" has been developed in search of better or more powerful musks of that type. However, since the Nitromusks have (generally) poor solubility, a tendency of discoloring under daylight and in combination with many common perfume or cosmetic chemicals, these musks have no great future in sight as the competition from the "Non-Nitro"-musks grows stronger every year.

It is interesting to note that the Butyryl derivative of one of the first "Non-nitro"-musks ever made (of the Tetralin family) was among the more pleasant smelling musks.

Prod.: from *tertiary*-Butyl-*meta*-xylol.

## 556: iso-BUTYRYL FORMALDEHYDE

An *alpha*-Ketoaldehyde, and a
higher homologue of Pyruvic aldehyde.

$(CH_3)_2CH—CO—CHO$

$C_5H_8O_2 = 100.12$

Colorless liquid. Slightly soluble in water, soluble in alcohol, Propylene Glycol and oils, also in Glycerin.

Powerful and diffusive, ethereal-creamy odor, in dilution just sweet and bland, but rather pleasant, caramellic dryout. Sweet, slightly buttery or creamy, but overall mostly caramellic taste. This material has been mentioned in perfumery literature for use in floral and sweet fragrance types, mainly as a part of a topnote complex.

It is rarely offered commercially, and it has not achieved any fame as a fragrance chemical at all.

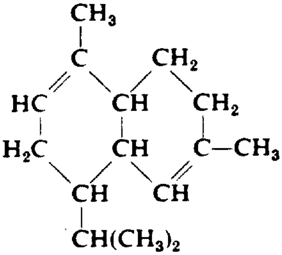
Its use in flavor compositions is limited to certain types of Caramel flavor.

Prod.: from Methyl-*iso*-butyl ketone.

3-297;

## 557: CADINENE

(There are at least 5 known isomers).
*3,4,5,8,9,10*-Hexahydro-*4-iso*-propyl-*1,6*-dimethylnaphthalene.
The structure of *alpha*-Cadinene is:



$C_{15}H_{24} = 204.26$

Colorless, slightly viscous liquid.
B.P. 275° C. Sp.Gr. 0.92.

Insoluble in water, soluble in alcohol, miscible with most perfume and flavor oils.

Mild, dry-woody, slightly medicinal-tarry odor with some similarity to spices or condiments (herbs) in the Cumin-Thyme family. Very stable to heat, alkali and organic acids.

Little, if any, of this chemical is used in perfume compositions as such. However, several chemical derivatives are used.

Occasionally used in flavor compositions, mostly as a fixative in candy flavors, where the stability to heat is an advantage. Concentrations of this chemical may then be as high as 4000 ppm in the finished candy.

Prod. by isolation from Brazilian Cedrela-wood oils or from the non-esterified portion of Amyris oil in the preparation of so-called "Amyris acetate".

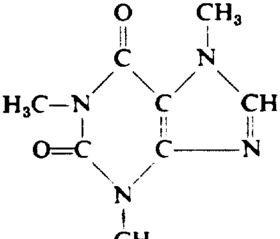
These isolates consist mainly of *alpha*-Cadinene. Isolation over the Dihydrochloride yields primarily *beta*-Cadinene.

G.R.A.S.

65-91; 67-639; 87-248; 86-28; 100-185;

## 558: CAFFEINE

Coffeine.
Theine.
Guaranine.
Methyl theobromine.
*1,3,7*-Trimethyl xanthine.
*1,3,7*-Trimethyl-*2,6*-dioxypurine.
"No-Doz" –
– and many other trade names for pharmaceutical purposes.



(anhydrous)

$C_8H_{10}N_4O_2 = 194.20$

White powder or hexagonal prisms (anhydrous) or silky needles (one Mol. $H_2O$). One Mol. water equals 8% of the material.

Soluble 2% in cold water, easily in hot water. Soluble 1,5% in alcohol.

Virtually odorless. Bitter taste, slightly woody-astringent.

Used in flavor work, rarely in the flavor oil itself (solubility problem) but as an additive to the finished product.

The concentration in certain carbonated beverages may be about 125 ppm. and it would take approximately one U.S.gallon of such soft drink to arrive at the equivalent of the maximum recommended daily dosage of Caffeine (0.50 grams). Five cups of good strong Coffee may contain a similar amount.

Prod. by isolation (extraction) from:

1) Tea dust (siftings).
2) Cocoa husks and shells.
3) Cola nuts.
4) Maté leaves.
5) Coffee beans - in the preparation of Caffeine-free Coffee.

Or it can be prepared synthetically from Dimethyl carbamide plus Malonic acid.

G.R.A.S. F.E.M.A. No.2224.

69-1669; 100-187; 124-372; 140-281;

## 559: CALCIUM ACETATE

Acetate of Lime.
"Sorbo-Calcion".

$Ca(CH_3COO)_2 - H_2O$

$C_4H_6CaO_4 - H_2O = 176.19$

White powder or granules or needles.

Soluble 33% in water. Slightly soluble in alcohol. Insoluble in perfume and flavor oils.

Decomposes when heated.

Virtually odorless, but hydrolysis by moisture yields mild acetic odor.

Sweet, bland taste.

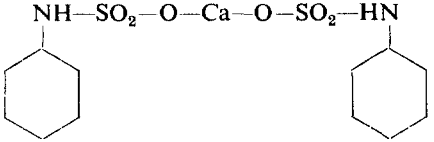
Used as an additive (sequestrant) to beverages and baked goods. Concentrations are about 200 ppm in beverages and up to 500 ppm in baked goods.

G.R.A.S. F.E.M.A. No.2228.

26-232; 100-190;

## 560: CALCIUM CYCLAMATE

Calcium cyclohexane sulfamate.
Calcium cyclohexyl sulfamate.
"Sucaryl Calcium".
"Cylan".
"Sucaryl" (Abbott) is a mixture of 10 parts Cyclamate and 1 part Saccharin.



(with 2 Mol. water of hydration)

$C_{12}H_{24}CaN_2O_6S_2 - 2H_2O = 432.58$

White crystals or crystalline powder. Virtually odorless.

Clean, sweet taste in water, about 30 to 40 times sweeter than cane sugar.

Soluble 20% in water - with acid reaction.

Soluble 40% in Propylene glycol.

Soluble 1.5% in alcohol. Insoluble in oils.

0.125 grams equal about 5 grams of cane suger in sweetening effect (about one teaspoon full).

Used extensively as a sweetening agent of no nutritional value, often in combination with Sodium saccharin. For all types of food, beverages, etc. and candy. Comparatively stable to heat.

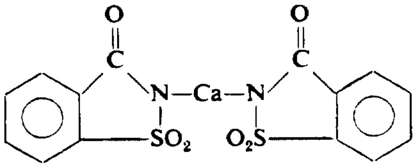
Prod. from Cyclohexane sulfamic acid (see this).

G.R.A.S.

100-308;

## 561: CALCIUM SACCHARIN

Calcium-di-*ortho*-benzosulfide.



+ 3½ $H_2O$

$C_{14}H_8CaN_2O_6S_2$, 3½ $H_2O$ = 467.49

White crystals or white crystalline powder.

Soluble 40% in water, poorly soluble in alcohol. Practically odorless.

Intensely sweet taste in water. Estimated potency of sweetness: 500 times cane sugar.

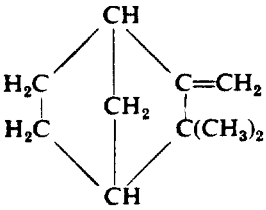
A non-nutritive sweetener, occasionally used in place of the Sodium salt. In spite of the fact that many Calcium salts have bitter taste, this salt is only sweet, and apparently not less so than the Sodium salt. Only high concentrations seem to leave the well-known "bitter aftertaste". This effect is compensated from by using low-potency sweeteners such as Sucaryl salts in combination with the Saccharin salts.

Prod. from Saccharin.

G.R.A.S.

## 562: CAMPHENE

Consists mainly of:
*2,2*-Dimethyl-*3*-methylene norbornane, or:
*3,3*-Dimethyl-*2*-methylene norcamphane.
The commercial product may contain up to 20% Tricyclene.



$C_{10}H_{16}$ = 136.24

Colorless, granular-crystalline, tenacious mass.
Sp.Gr. 0.84 (liquid). B.P. 159° C.
M.P. 51° C.

Sublimes when heated. Insoluble in water, soluble in alcohol, miscible with most oils.

Mild, oily-camphoraceous odor, with little or no "warm-cold-feel" as one can observe with Camphor.

Terpeney-camphoraceous taste, remotely resembling that of Celluloid (if the reader has ever tasted that!).

Extensively used in Pine, Lavender, Lavandin, Cedar and Citrus fragrances, particularly those of lower cost and high volatility. Camphene is very inexpensive and gives a "lift" to the above fragrance types, often desirable in household product perfumes, detergent fragrances, etc., where tenacity may even be undesirable. It constitutes an important item in artificial essential oils, not only Lavandin and Pine Needle.

Used in Spice and Nutmeg flavor compositions, partly in reconstituted spice oils, partly in general as a "lift" to the flavor composition.

The concentration in candy may be as high as 150 to 175 ppm.

G.R.A.S. F.E.M.A. No.2229.

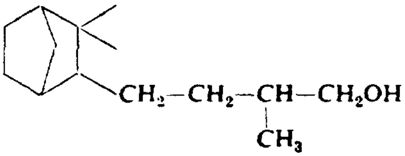
Prod. (several methods) e. g. 1) from *alpha*-Pinene via the Hydrochloride by alkali to Camphene. Or 2) from *beta*-Pinene via Nopol to Camphene (catalytic isomerization).

The synthesis of Camphene is over 100 years old.

26-448; 65-66; 67-583; 31-8; 87-179; 100-200; B-V-156;
(Glidden Co., datasheet, May 1, 1961).

## 563: 3-(iso-**CAMPHENYL**-8)-2-**METHYLPROPANOL**-1

The commercial product contains also:
*3*-(Camphenyl-*8*)-*2*-methylpropanol-*1*.



$C_{14}H_{26}O = 210.36$

- and one or more isomers.

Viscous, almost colorless or very pale straw-colored liquid. Insoluble in water, soluble in alcohol and oils.

The commercial product is not marketed as a single chemical or sold under its proper chemical name. Various perfume specialties are available under trade names, and they are based upon the title chemical with variable amounts of isomers and trace additives for bouquetting.

The odor of the chemical itself is sweet, woody and very tenacious. The wood-note has resamblance to Sandalwood, but is not quite as sweet. In fact, it has also some similarity to Cedarwood oil.

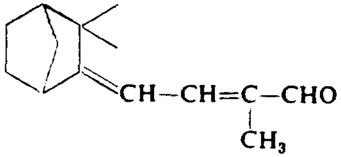
The specialty is recommended for use in modern Sandalwood or wood fragrance types for Men, or Oriental compositions for women's fragrances. It seems to perform best when Sandalwood oil (natural) is present, but it can also be blended with good effects with Butylcyclohexylacetate, Methylionones, Vetiver oil, Oakmoss, etc.

In the author's opinion, it is not the most successful Sandalwood chemical.

Prod.: by hydrogenation of the aldehyde, which is manufactured according to German patent No. 34.195 of 14th Aug. 1963, DWP.

See also: *iso*-Bornyl methoxy cyclohexanol.

## 564: 3-(**CAMPHENYL**-8)-2-**METHYLPROPEN**-3-**AL**



$C_{14}H_{20}O = 204.31$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Green-woody, moderately sweet and very tenacious odor.

This aldehyde has been suggested for use in perfume compositions mainly as a novel note in modern woody and woody-green fragrance types.

It is, to the author's knowledge, not available under its proper chemical name, and it does not seem to be used in significant quantities at all.

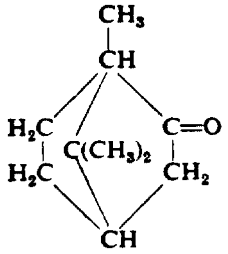
The corresponding alcohol, which is also marketed under a trade name (usually in the form of a mixture of isomers with trace additives of bouquetting materials) is more interesting as a Sandalwood type fragrance chemical.

Subject aldehyde could find use in Chypre and Fougere types, since it blends well with Oakmoss, Salicylates, Vetiver, Patchouli, Butylcyclohexyl acetate and the Ionones.

Prod.: German patent No. 34195 DWP, Aug. 14, 1963.

## 565: dextro-**CAMPHOR**

*2*-Camphanone.
Japancamphor.
*1,7,7*-Trimethylbicyclo (*2,2,1*)-*2*-heptanone.
*2*-Keto-*1,7,7*-trimethylnorcamphane.
(The *dextro*-rotatory form is required by the U.S. Pharmacopoeia, but this form constitutes only a small part of the total production of Camphor in the U.S.A., where the bulk is the racemic form).



$C_{10}H_{16}O = 152.24$

Grainy-crystalline translucent mass, or grainy crystals. Volatile with steam, sublimes when heated. Sp.Gr. 0.992.
M.P. 179-180° C. B.P. 208° C.
Soluble 0.12% in water, 50% in alcohol, miscible with most oils. Warm-minty almost ethereal-diffusive odor of very low tenacity. Slightly bitter warm, then cool taste.

Occasionally used in perfume compositions, more often in artificial essential oils of the Lavender-Lavandin-Spike family. Also in certain types of masking odors for industrial purposes.

Used in flavor compositions, mainly in mint flavors as a "lift" and as a modifier.

The concentration in the finished product may be about 25 ppm.

Note: Camphor forms explosive vapors with air.

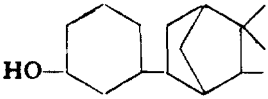
Prod.:
1) Naturally isolated from distilled Camphor wood oil.
2) Synthetic from Vinyl chloride cyclopentadiene (mainly in Germany).
3) From Pinene (mainly in the U.S.A.).

G.R.A.S. F.E.M.A. No.2230.

26-448; 31-90; 85-39; 89-290; 100-200; B-VII-101; 140-168;

## 566: 3-(iso-CAMPHYL-5)-CYCLOHEXANOL

*meta*-(*iso*-Camphyl-*5*)-cyclohexanol.



$C_{16}H_{28}O = 236.40$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol, miscible with oils.

Very tenacious, mild Sandalwood type odor, not as sweet or balsamic as Sandalwood oil, and not nearly as powerful in active use.

This material, rarely offered under its chemical name, is used in perfume compositions for its Sandalwood character and economical stability.

Like *iso*-Bornyl metoxycyclohexanol, this alcohol is mainly used in conjunction with true Sandalwood oil. Proportions up to 50/50 are normally acceptable as general replacement for Sandalwood oil, but there are cases where the natural oil cannot be substituted by any single chemical, at least not at a 50/50 proportion.

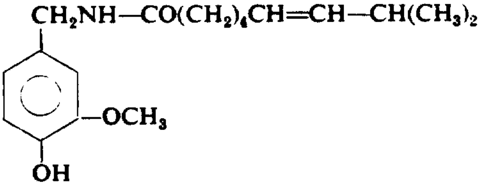
Literature has pointed out that the *2*- and *4*-isomers (*ortho*- and *para*-) are of little or no perfumery value.

Prod.: from Resorcinol and *iso*-Borneol (from *beta*-Pinene), followed by hydrogenation.

(Firmenich pat. appl. Sept. 1, 1964).

## 567: CAPSAICINE

*iso*-Decenoic acid, Vanillylamide.
*8*-Methyl-*N*-vanillyl-*6*-nonenamide.
7-Methyloct-*5*-ene-*1*-carboxylic acid, Vanillylamide.
(A pungent principle occurring in Capsicum).



$C_{18}H_{27}NO_3 = 305.42$

Monoclinic, rectangular crystal scales or plates. M.P. 65° C.

Insoluble in water at room temp. – slightly soluble in warm water. Soluble in alcohol and oils.

Burning-pungent taste at 10 ppm with perceptible pungency down to 0.09 ppm (subjective evaluation).

Peculiar mild, warm-herbaceous odor, overall weak.

Used extensively in spice blends to increase pungency of the blend or its components (Ginger, etc.). In Pepper blends, meat sauces, pickle flavors, Ginger ale soft drink flavor (in certain countries an excessive pungency is requested), etc.

See also comments under NONANOYL VANILLYLAMIDE.

NOTE: Although C. is a phenol, it is not inactivated by alkali, and it maintains its pungency under alkaline conditions (diff. from the pungency of Ginger).

Prod.: synth. from Vanillylamine and *iso*-Decenylchloride.

1-843; 26-450; 30-182; 68-732; 100-205; 104-122; 124-278; 130-505; 158-209; B-XIII-322, erstes Ergzbd.

## 568: CARBON DISULFIDE

Dithiocarbonic anhydride.

$CS_2 = 76.14$

Colorless mobile liquid. B.P. 46° C. Sp.Gr. 1.26.

0.3% soluble in water. Miscible with alcohol and oils.

Extremely volatile. Diffusive odor, chokingly repulsive, ethereal-sulfuraceous. It has often been claimed that the malodor is due entirely to impurities, and the author can confirm that this chemical, coming out of the exhaust vent of a Gaschromatograph, does not smell truly repulsive, but rather sweet, cabbage-like, almost herbaceous, slightly green.

Since Carbon disulfide has been used for certain extraction purposes it is included in this handbook. Also because it may actually have an interesting odor when absolutely pure.

NOTE: Carbon disulfide is extremely poisonous and flammable. Vapors form explosive mixtures with air. At 1% concentration, the mixed vapors may ignite upon contact with a hot steampipe.

Naturally occurring in essential oil of Black Mustard Seed.

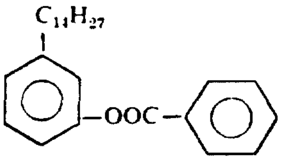
Prod. from:

1) Charcoal with Sulfur vapors.
2) Methane with Sulfur vapors.

26-450; 30-233; 90-793; 100-211; B-III-197;

## 569: CARDANYL BENZOATE

The commercial product consists mainly of the *meta*-isomer with the *para*-isomer as a minor impurity.



(*meta*-)

$C_{27}H_{36}O_2 = 392.59$

Colorless viscous liquid. Insoluble in water, soluble in alcohol, miscible with oils, but not in all proportions.

Dry, but pleasant "Russian-leather" type of considerable tenacity.

This material, rarely offered commercially, has found a little use in fragrances where a "non-phenolic" or "non-medicinal" type of Leather odor is called for, e. g. in the refined "Cuir" bases, ect. It is free from tarry notes, and the dry character is actually accompanied by considerable sweetness in the terminal notes.

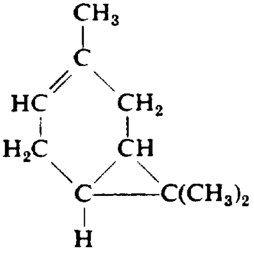
It is quite possible that one isomer has a more desirable odor than the other, but the author has not yet seen the purified isomers.

Prod. by Benzoylation of Cardanol, a phenol isolated from the oil of the Cashew-nut shell.

30-421; 31-25; 159-624;
See also notes under: Dihydrocarveol and Dihydrocarvyl benzoate.

## 570: Δ3-CARENE

*iso*-Diprene.
*3,7,7*-Trimethyl bicyclo-*0,1,4*-hepten-*3*.
A number of isomers are known:
*d-Δ3*-Carene.
*dl-Δ3*-Carene.
*l-Δ3*-Carene.
*l-Δ4*-Carene. (synthetic).
*d-Δ4*-Carene. (natural).
But only a few have attained enough interest to become regularly manufactured items (*Δ3*-Carene and *Δ4*-Carene).



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 165° C.

Practically insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol, miscible with oils.

Sweet, duffusive, penetrating odor, somewhat reminiscent of a refined Limonene.

(The *Δ4*-Carene has a *para*-Cymene-like odor).

This terpene is unstable when exposed to air.

Used mainly in the "reconstruction" of essential oils, such as Spearmint, Lemon, Lime, etc. Also as an intermediate in the manufacture of perfume chemicals by Formaldehyde condensation process.

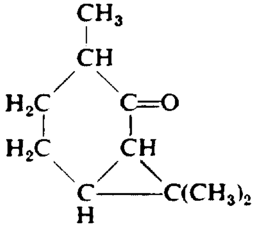
Prod. either synthetically or by isolation from Turpentine fractions.

G.R.A.S.

65-49; 67-512; 86-29; 87-118; (The Glidden Co., info. sheet to author).
Also: Camphor & Allied Products, Ltd., Bombay-1, India.

## 571: CARONE

*5*-Ketocarane.
(both *dextro*- and *laevo*-forms have been synthesized).



$C_{10}H_{16}O = 152.24$

Colorless mobile liquid. B.P. 210° C.
Sp.Gr. 0.96.

Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, yet refreshing odor. Very volatile (poor tenacity).

Occasionally used in the "reconstruction" of essential oils.

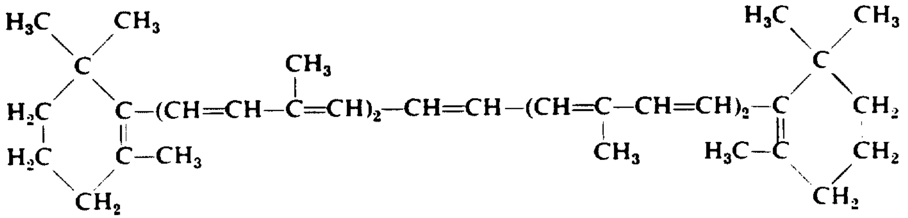
Prod. from Carvone via Dihydrocarvone, reacted with HBr followed by treatment with alcoholic Potassium hydroxide.

65-447; 67-560;

## 572: beta-CAROTENE

*trans-beta*-Carotene.
*1,18-bis*(*2,6,6*-Trimethyl cyclohexen-*6*-yl)-*3,7,12,16*-Tetramethyl-octadecanonaene.

One of the Provitamins A.
One gram of *beta*-Carotene equals approximately 1,600,000 units of Vitamin A activity.



$C_{40}H_{56} = 536.85$

Crystals of dark orange color.
M.P. 176-182° C.

Insoluble in water. Soluble 1 to 6% in various vegetable oils, 4% soluble in chloroform.

Decomposes when exposed to air, particularly warm air.

Limited stability under $CO_2$ at room temperature.

Extensively used for coloring of foods. The material is virtually without odor at the concentration used for coloring purposes.

However, Carotene has been suggested for use in Violet fragrances. Although this may sound very odd, there is an interesting connection between *beta*-Ionone and *beta*-Carotene, the Ionone being an intermediate step in the synthesis of Carotene.

It is also interesting to note the very perceptible odor of "Violets" (Ionones) emanating from piles of fruitclusters of the Guinea oil palm. The fruits contain *beta*-Carotene and may also contain Ionone leftover from Nature's synthesis of the Provitamin.

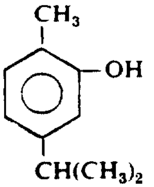
This hydrocarbon has no practical interest to creative perfumery.

G.R.A.S.

1-722; 4-28; 100-216;
See also: Hoffmann-laRoche "The Color That Nourishes" (Brochure), and: Food Technology, vol. XII, October 1958.

## 573: CARVACROL

*2-para*-Cymenol.
*2*-Methyl-*5*-*iso*-propylphenol.
*iso*-Thymol.
Cymophenol.
*2*-Hydroxy-*para*-cymene.
*iso*-Propyl-*ortho*-cresol.



$C_{10}H_{15}O = 151.23$

Colorless liquid. Very slightly soluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Solidifies in the cold, M.P. 1° C.
B.P. 238° C. Sp.Gr. 0.98.

Penetrating, dry-medicinal ("phenolic") – herbaceous odor with a spicy undertone. Main difference from Thymol odor is the lack of sweetness in Carvacrol, the latter being more "tarry".

Used in perfume compositions, mainly in industrial fragrances, certain types of "heavy-duty" household fragrances, soap perfumes, etc. It has good power, and is fairly stable in ordinary soaps, in spite of its hydroxyl-group (phenol radicle).

Used in flavor compositions, mainly in spice and meat flavors, Citrus compositions, Mint flavors, etc. Furthermore as a modifier in certain types of Mouthwash flavor.

Concentrations in the finished product may be about 125 ppm. in baked goods, somewhat lower in other products.

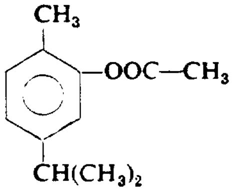
Prod. (several methods) e. g. by sulfonation of *para*-Cymene to *para*-Cymene-*2*-sulfonic acid, followed by alkali fusion. Thymol is a by-product in that synthesis.

G.R.A.S. F.E.M.A. No.2245.

4-28; 26-452; 30-420; 31-24; 31-143; 65-503; 68-421; 85-45; 86-29; 90-394; 95-115; 96-93; 100-527; B-IV-527; 140-169;

## 574: CARVACRYL ACETATE

*2*-Methyl-*5*-*iso*-propyl acetylphenol.



$C_{12}H_{16}O_2$ = 192.26

Colorless or pale yellowish liquid.

B.P. 246° C. Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Aromatic-mild odor, very tenacious and somewhat reminiscent of the odor of Carrot seed.

Occasionally used in perfume compositions for Fougère, Carnation, Clover, Sweet Williams, etc. as a modifier for other spicy notes. It seems to take the rough chemical character out of *iso*-Butyl- or Amyl salicylate in such compositions.

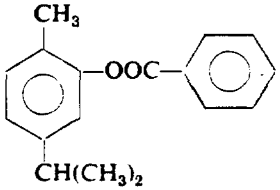
This ester is, to the author's knowledge, not commonly used in flavor work.

Prod. by acetylation of Carvacrol with Acetic anhydride.

4-28; 90-570;

## 575: CARVACRYL BENZOATE

*2*-Methyl-*5*-*iso*-propyl benzoylphenol.



$C_{17}H_{18}O_2$ = 254.33

Pale straw-colored, viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, but very tenacious odor, reminiscent of the Fougere-theme, mild-herbaceous, sweet-woody with a faintly medicinal undertone.

Suggested for use as an additive for Oakmoss, a blender or modifier in Fougere compositions.

However, this ester is not regularly available from the usual manufacturers of perfume chemicals.

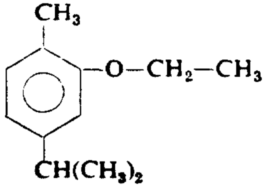
Prod. from Carvacrol and Benzoylchloride.

86-29;

## 576: CARVACRYL ETHYLETHER

Ethylcarvacrol.

*2*-Ethoxy-*para*-cymene.



$C_{12}H_{18}O$ = 178.28

Colorless liquid. Slightly soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Warm-spicy-herbaceous odor, somewhat reminiscent of the odor of Carrot seed, sweeter than the odor of Carvacryl acetate.

Used in spice flavor compositions as a modifier and sweetener for Carvacrol (if this phenol is used).

Concentrations may be as high as 40 ppm in the finished product.

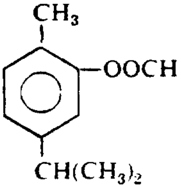
G.R.A.S. F.E.M.A. No.2246.

Prod. from Carvacrol with Diethylsulfate in cold weak aqueous alkali solution.

31-143; 86-29;

## 577: CARVACRYL FORMATE

2-Methyl-5-*iso*-propyl formylphenol.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Very slightly soluble in water. Soluble in alcohol and oils.

Green-spicy, "vegetable" type of odor, more interesting than that of the acetate.

Has been suggested for use in Fougere and Chypre fragrance types.

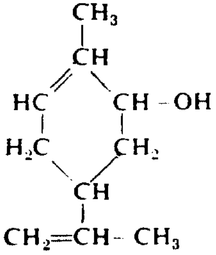
Could possibly find use in spice flavor blends, seasoning flavors, condiments, pickle flavoring, etc.

Prod. from Carvacrol with HCOCl (in the form of HCl plus CO) in the cold.

## 578: laevo-CARVEOL

*laevo-para*-Mentha-6,8-dien-2-ol.
*1*-Methyl-4-*iso*-propenyl cyclohexen-6-ol-2.

Of the 6 isomers, the *cis-laevo*-Carveol is the most interesting at the time of writing this monograph. It is considered a natural component of Spearmint oil.



$C_{10}H_{16}O = 152.24$

Colorless liquid. (*cis-dextro*-isomer has M.P. 25° C.) B.P. 227° C. Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils.

The odor is more Caraway-like than Spearmint-like (according to the majority of opinions).

This alcohol finds use in flavor compositions to support the flavor of Mint, Spearmint, Caraway or spice flavors or flavor blends.

The concentration in finished product will be about 25 ppm. (Candy).

G.R.A.S. F.E.M.A. No.2247. (The Federal Register does not discriminate between the various stereo-isomer forms).

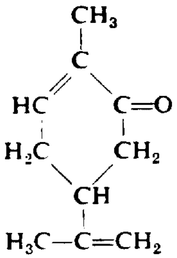
Prod.:

1) from Limonene by oxidation.
2) from *laevo*-Carvone by reduction with Lithium Aluminium hydride.

65-203; 67-521; 88-114; 89-260;

## **579:** dextro-**CARVONE**

*6,8*-(or *9*)-*para*-Menthadien-*2*-one.
*d*-*1*-Methyl-*4*-*iso*-propenyl-*6*-cyclohexen-*2*-one.
"Carvol" (old, misleading name).



$C_{10}H_{14}O = 150.22$

Colorless or pale straw-colored mobile liquid. Darkens upon exposure to air and daylight. Sp.Gr. 0.97. B.P. 230° C.

Insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, breadlike, spicy and slightly floral odor, reminiscent of Caraway seed or Dill seed.

Warm, sweet, spicy-herbaceous, breadlike taste.

Occasionally used in perfumes, but the *laevo*-Carvone is often preferred here.

Used in flavor compositions as a fortifier for Caraway seed oil or Dill oil seed (in which oils this ketone is a major component). Since this isomer is rarely offered in the synthetic form, it has not become as popular as the *laevo*-Carvone. The use of Caraway-Dill flavor is confined to a few, although by volume very large, commercial products (Bread, Pickles, Spices, etc.).

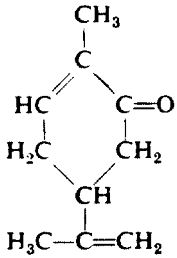
Prod.:
1) Synthetic: no commercial scale production.
2) Isolation: From Caraway seed oil or Dill seed oil.

G.R.A.S. F.E.M.A. No.2249 (no discrimination between *dextro-* and *laevo*-Carvone).

65-412; 89-250; 100-217; 104-125;

## **580:** laevo-**CARVONE**

*l*-*1*-Methyl-*4*-*iso*-propenyl-*6*-cyclohexen-*2*-one.
*para*-Menthadien-*6*,*8*(*9*)-one-(*2*).



$C_{10}H_{14}O = 150.22$

Colorless liquid (synthetic product only, the isolated is pale yellowish). Insoluble in water, soluble in alcohol and oils. Fairly soluble in Propylene glycol. B.P. 231° C. Sp.Gr. 0.96.

Warm-herbaceous, breadlike, penetrating and diffusive odor, somewhat spicy, in extreme dilution also floral, overall reminiscent of Spearmint oil (rectified).

Warm and sweet, spicy, refreshing minty taste.

Occasionally used in perfume compositions, particularly in floral bases, where it introduces enormous power and often lends pleasing natural notes to the fragrance. However, it demands great skill and experience in application. It seems to constitute a very good and compatible companion to Rose Oxide and the Jasmone chemicals.

Extensively used in flavor compositions, mainly as a powerful Spearmint note, to fortify Spearmint oil, etc. in hard candy, chewing gum, toothpaste and many kinds of candy. Furthermore in Mint flavor blends, spice blends, liquor flavors, etc.

Concentration may be about 800 ppm in beverages, but may reach 3000 ppm or more in toothpaste and almost a similar level in chewing gum.

Synthetic *laevo*-Carvone is marketed at well below the price of that of a good grade Spearmint oil at the time of writing this monograph.

Prod.:

1) Synthetic: from *dextro*-Limonene via the Nitrosylchloride (several patented methods).
2) Isolated: Very rarely – from Spearmint oil, not commercially feasible.
3) from alpha-Pinene oxide via Sobrerol and Carvylacetate.

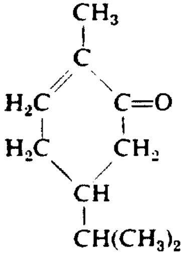
G.R.A.S. F.E.M.A. No.2249 (no discrimination between *dextro*- and *laevo*-Carvone in this reference work).

NOTE: *laevo*-Carvone constitutes an intermediate step in the oxidation of *d*-Limonene in sweet Orange oil. The off-odor in sweet Orange oil is often due to traces of *laevo*-Carvone which will eventually oxidize further to Carvacrol and further impair the odor of the Orange oil.

65-412; 89-250; 100-217; 85-45; 104-590; 140-167; Glidden 1966;

## 581: CARVOTANACETONE

*para*-Menthen-*6*-one-*2*.
*1*-Methyl-*4*-*iso*-propyl cyclohexen-*6*-one-*2*.
3 stereo-isomers of interest:
*dextro*-
*laevo*-
*dl(racemic)*-



$C_{10}H_{16}O = 152.24$

Colorless or pale yellowish oily liquid.
B.P. 228° C. Sp.Gr. 0.935.

Insoluble in water, soluble in alcohol and oils.

Warm, herbaceous-spicy odor, reminiscent of Carvone, with less character.

Spicy-herbaceous, but somewhat bitter taste.

Very rarely used in perfumes or flavors.

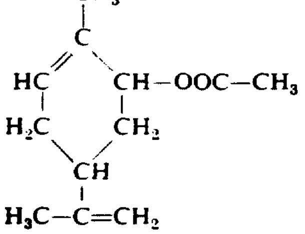
Prod.:

1) by isolation from the essential oil of Blumea malcolmii.
2) synthetically from Thujone.

65-406; 67-525; 89-225;

## 582: laevo-CARVYL ACETATE

*l-para*-Mentha-*6*,*8*-dien-*2*-yl acetate.
The *trans*-isomer is considered natural component of Spearmint oil.



$C_{12}H_{18}O_2 = 194.28$

Colorless, slightly oily liquid. Very slightly soluble in water, soluble in Propylene glycol, alcohol and oils. Sp.Gr. 0.97. B.P. 229° C.

Refreshing, green-minty, Spearmint-like odor, more "cool" than Carvone, not as penetrating, but with a peculiar "metallic" undertone.

Sweet spicy-minty, green and refreshing taste, not as powerful as Carvone, but overall more pleasant, versatile in character.

Used in flavor compositions; increasingly used since it is now a commercially available item. For mint compositions, artificial mint oils, spice blends, meat flavors, etc.

This ester is much more stable under air-exposure than the Carvone, and this fact opens wide fields of application for the ester. The concentration in Ice-cream, for example, may be as high as 40 ppm. Carvone would break down quickly in such aerated product.

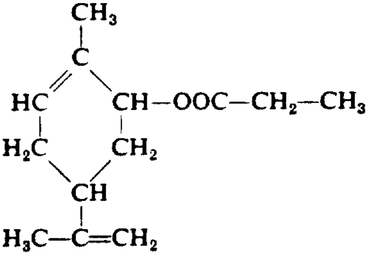
Prod. by direct esterification of *laevo*-Carveol with Acetic anhydride and Sodium acetate. It can also be prepared directly from *alpha*-Terpinyl acetate.

G.R.A.S. F.E.M.A. No.2250.

(Fritzsche Bros.. Co. info.); 88-116; 90-295;

## 583: laevo-CARVYL PROPIONATE

*l-para*-Mentha-*6*,*8*-dien-*2*-yl propionate.



$C_{13}H_{20}O_2 = 208.30$

Colorless, slightly oily liquid. B.P. 239° C. Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils.

Sweet, warm, minty-spearminty, warmer and more herbaceous than the acetate, also displaying a slightly fruity undertone. Sweet, herbaceous-fruity-minty taste.

Occasionally used as a modifier for the acetate in mint flavor compositions, particularly for candy.

The concentration in the finished product may be about 25 ppm.

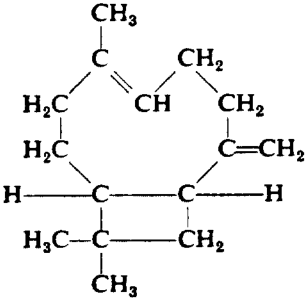
G.R.A.S. F.E.M.A. No.2251.

Prod. by direct esterification of *laevo*-Carveol with Propionic anhydride. Also from *alpha*-Terpinyl propionate.

(Fritzsche Bros. Co. Inc., info & sample).

## 584: beta-CARYOPHYLLENE

(commercially known as "Caryophyllene"). (*alpha*-Caryophyllene, also known as Humulene, accompanies *beta*- in Nature).



$C_{15}H_{24} = 204.36$

Colorless oily liquid. Sp.Gr. 0.90. B.P. 256° C.

Woody-spicy, dry and tenacious odor. Many descriptions include the word "clove-like", but the author finds that the typical "Clove-odor" is to be found only in Clove bud oil and Clove bud absolute – apart from the dried Clove buds proper. And in those products one will find fresh-fruity, creamy, slightly green notes in the non-Eugenolic-portion. One test on Clove oil uses Magnesium carbonate upon which you drop a few drops of Clove bud oil. If the wet mass smells of Clove after several hours, one is allowed to conclude that this was Clove oil and not just Eugenol. However, there is little, if any, Caryophyllene in the named products, and the Clove-like odor must derive from chemicals other than that hydrocarbon.

Dry-woody, somewhat bitter taste. It is true that there is a similarity to Clove leaf oil, but that oil does contain Caryophyllene and includes it in its odor picture.

Occasionally used in perfume compositions, but the modern derivatives of Caryophyllene are more and more preferred. See following two monographs.

Used in flavor compositions, mainly in spice blends and particularly for chewing gum, where concentrations may be as high as 200 ppm. It also acts as a fixative for the more volatile spice chemicals such as Cinnamic aldehyde, etc.

G.R.A.S. F.E.M.A. No.2252.

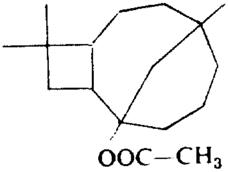
Prod. by isolation from Clove leaf oil, Clove stem oil or Cinnamon leaf oil.

Also obtained from certain fractions of American Pine oil. That Caryophyllene is not exclusively a *beta*-Caryophyllene, and it often carries an unpleasant off-odor of sulfuraceous character (from Sulfate Turpentine, etc.).

6-149; 65-99; 87-283; 67-651; (Arizona Chemical Co.).

## 585: CARYOPHYLLENE ACETATE

Caryophyllene Alcohol acetate.
The acetate of a sesquiterpene alcohol, derived from Clove-Caryophyllene.



$C_{17}H_{28}O_2 = 264.41$

Practically colorless, slightly viscous liquid. Sp.Gr. 0.99-1.00.

Insoluble in water, soluble in alcohol and oils.

Mild fruity-woody odor, fresh-green, sap-like, quite tenacious.

Could possibly find use in perfumery if it were made available in steady quantities at comparatively low cost, so that soap perfumes could be prepared with this ester.

Used as a fixative in flavor compositions.

The concentration is about 25 ppm. in Candy, while it may be as high as 150 to 175 ppm. in chewing gum.

G.R.A.S.

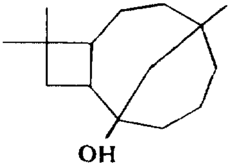
Prod. by direct Acetylation of Caryophyllene alcohol (see next monograph).

(Several perfume specialties marketed under trade names are basically this ester).

6-150;

## 586: CARYOPHYLLENE ALCOHOL

*beta*-Caryophyllene alcohol.
(Not to be confused with Caryophyllene glycol, a dihydric, tricyclic alcohol produced by mild acid reaction upon Caryophyllene oxide (hydration by catalyst)).



$C_{15}H_{26}O = 222.37$

Solid crystalline mass, insoluble in water, soluble in alcohol, miscible with most perfume oils.

Warm, earthy-mossy, spicy odor, remotely resembling that of Trimethyl cyclohexanol, slightly minty, basically woody, and of good tenacity.

Suggested for use in perfume compositions, where it might well act as a fixative and at the same time introduce interesting new "dry" notes, tobacco-like, spicy-mossy. It blends excellently with Oakmoss products, Geranium, Vetiver, and Patchouli oil. Its peculiar combination of notes fits very well in the Hyacinth picture, although this alcohol really is not a floral chemical.

Used in flavor compositions, mainly for mushroom flavors. The concentration may be about 50 ppm. in the finished product.

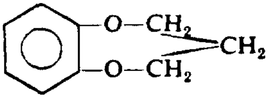
G.R.A.S.

Prod. from Clove-Caryophyllene by hydration (cyclization) with mineral acid in the cold.

6-150; 65-102; 67-657; 87-286; 88-338; (Fritzsche Bros. info. & sample).

## 587: CATECHOL CYCLO-TRIMETHYLENE ETHER

Pyrocatechin trimethylene ether, cyclic.



$C_9H_{10}O_2 = 150.18$

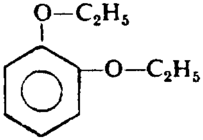
Reported as being a potential perfume chemical with distinctly floral note.

Prod. from Pyrocatechol sodium plus Trimethylene dibromide followed by reaction with Sodium in Methanol.

31-153;

## 588: CATECHOL DIETHYLETHER

*ortho*-Diethoxy benzene.
Diethylcatechol (misleading name).
Pyrocatechin diethylether.



$C_{10}H_{14}O_2 = 166.22$

White crystals. Practically insoluble in water, soluble in alcohol and oils. M.P. 44° C.

Sweet Vanilla-like odor, weaker than Vanillin, but a heavier note with a trace of Anisic sweetness in it.

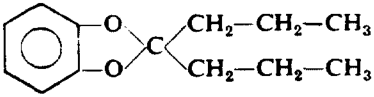
Suggested for use in perfumes, but does not seem to offer sufficiently of interesting notes or power. Vanillin - Ethylvanillin (so-called), Veratraldehyde, etc. cover the perfumer's need for Vanilla-like notes.

Prod. from Pyrocatechol by Ethylation with Diethyl sulfate in cold aqueous alkali.

31-146; 68-467;

## 589: CATECHOL DI-n-PROPYL KETAL

Di-*n*-propyl catecholketal.
Pyrocatechin di-*n*-propylketal.



$C_{13}H_{18}O_2 = 206.29$

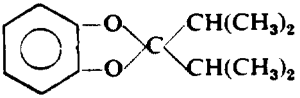
Reported as being an interesting perfume chemical with Geranium-Rose type odor, somewhat sweeter than that of the *iso*-propylketal.

Prod.: From Catechol by condensation with Di-*n*-propylketone.

31-117;

## 590: CATECHOL DI-iso-PROPYL KETAL

Pyrocatechol di-*iso*-propylketal.



$C_{13}H_{18}O_2 = 206.29$

Reported as being an interesting perfume chemical with a conspicuous Rose-geranium type odor.

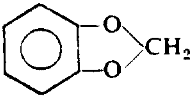
The Di-*n*-propyl ketal is also known (similar odor).

Prod.: From Pyrocatechol plus Di-*iso*-propyl ketone.

30-253; 31-117; Agfa data sheet; 159-416;

## 591: CATECHOL METHYLENE ETHER

566. CATECHOL METHYLENE ETHER
Pyrocatechol monomethylene ether.
*1,2*-Methylene dioxybenzene.



$C_7H_6O_2 = 122.13$

Colorless liquid. Sp.Gr. 1.19. B.P. 172° C.

Pleasant, sweet, floral odor, remotely resembling Anise and Heliotrope, but more diffusive and of poor tenacity.

Commercial samples of doubtful purity show harsh Anisole-like odor.

Suggested for use in perfume compositions, but its high vapor pressure at room temperature makes it somewhat difficult to "control", particularly since it cannot be applied in very high percentage, being of a rather unusual odor type.

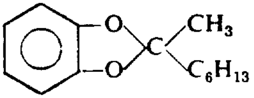
Prod.:

1) from Pyrocatechol plus Methylene chloride with Sodium ethoxide in Ethyl alcohol.
2) from Pyrocatechol in weak aqueous Sodium hydroxide solution with Methylene iodide.

68-468; 72-66;

## 592: CATECHOL METHYL HEXYL KETAL

Pyrocatechin methyl hexyl ketal.
"Methyl hexyl ketal".



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-floral, herbaceous, Jasmin-like odor of good tenacity.

This ketal, one of many ketals developed from Catechol since the 1930's when a few of these new materials were marketed under trade names, has remained on the shelf in many perfume laboratories. Its odor offers an excellent extender to the odor of Amylcinnamic aldehyde in that it is more floral, less tenacious, less oily, but equally versatile and adjusts well to many floral fragrance types.

If it were manufactured on a large scale, its price could undoubtedly be brought down within the attractive limits for use in everyday perfumery.

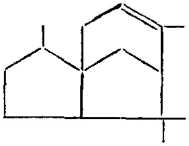
It blends also well with Amylsalicylate, Hydroxycitronellal, Heliotropine, Linalool, etc. and it is stable in mild alkali.

Prod.: from Catechol and Methyl hexyl ketone by condensation.

(See also: 31-118).

## 593: CEDRENE

The commercial product is mainly *alpha*-Cedrene.



$C_{15}H_{24} = 204.36$

Colorless oily liquid. B.P. 262° C. Sp.Gr. 0.93.

Insoluble in water, soluble in alcohol and perfume oils.

Woody-camphoraceous, somewhat dry and green odor, reminiscent of Cedarwood (American).

Fractions from American Cedarwood oil, rich in Cedrene, are used in perfumery mainly for soaps, household products and in industrial perfumes, masking odors, etc.

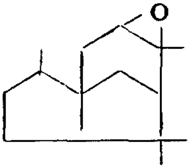
This sesquiterpene is the main component of "Eastern" or "Virginia" Cedarwood oil and is in fairly good supply, but at times insufficient to allow for this material to go into real large volume perfumery. Many interesting perfume materials are manufactured from Cedrene, and this puts a certain limit to the availability of the hydrocarbon.

The second-largest component of Virginia Cedarwood oil, Cedrol, is in lesser demand, and this is why one method of increasing the volume of Cedrene utilizes the Cedrol and converts it into the terpene.

Prod.: by fractionated distillation of Eastern American Cedarwood oil, or: from Cedrol by dehydration.

65-116; 67-651; 87-311;

## 594: alpha-CEDRENE EPOXIDE



$C_{15}H_{24}O = 220.36$

Colorless viscous liquid. Insoluble in water, soluble in alcohol and perfume oils.

Dry-woody, but very pleasant odor with a certain sweetness in its undertone. The combination of dry and sweet notes is rare and found only in a few natural wood oils, in Ambergris and in certain herbaceous extracts.

Blends excellently with Oakmoss, Methylionones (particularly the so-called *delta*-Methylionone, or *iso*-Methyl *beta*-Ionone), Labdanum extracts, Methylcoumarins, etc.

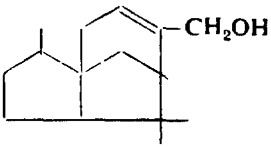
Chemical perfumery research has had the eyes fixed upon "Oxides" or Epoxides for a very long time. Other examples of Terpenes with corresponding Epoxides of perfumery interest are:

Carene – Epoxycarene
Caryophyllene – Epoxydihydrocaryophyllene
Pinene – Pinol
Menthane – Cineole
etc.

not to mention the Epoxides related to certain alcohols (Linalool oxide, "Rose oxide" etc.).

## 595: CEDRENOL

(*primary*-Cedrenol)



$C_{15}H_{24}O = 220.36$

White crystals (in the pure state) or:
Viscous liquid with considerable crystalline deposit, liquid is pale straw colored (lower grade products).

Crystals: M.P. 104° C. B.P. 270° C.
Sp.Gr. 1.01 (liquid).

Insoluble in water, soluble in alcohol, miscible with perfume oils. Used as a fixative in soaps and "heavy-duty" perfume types. The odor varies with the purity, since traces of Cedrene and other impurities heavily influence the odor picture. Generally of mild woody odor, less dry, more balsamic than the Cedrene. The tenacity is good, but the actual "odor value" is unimpressive.

Prod.:

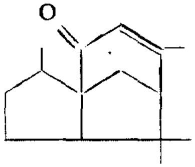
1) by isolation from Virginia Cedarwood oil (fractions higher than Cedrene).
2) By oxidation of Cedrene via Cedrenyl acetate. By this process one can obtain either *primary* or *secondary* Cedrenol.

As mentioned under Cedrene, the process of converting Cedrene into Cedrenol is contrary to commercial interest.

65-283; 67-651; 88-329;

## 596: CEDRENONE

Sometimes called "Cedrone".
The ketone corresponding to the *secondary*-Cedrenol.



$C_{15}H_{22}O = 218.34$

Pale yellowish or straw-colored viscous liquid with considerable deposit of crystals, or, if pure, almost white crystals of M.P. 33° C. B.P. 264° C. Sp.Gr. 1.01. (liquid).

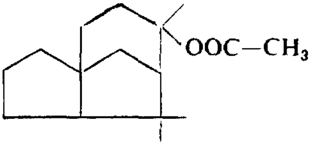
Occasionally used as a fixative in soap perfumes. Its soft-woody odor is quite tenacious but without much character or distinction.

Prod. from Cedrenol by Chromic acid oxidation.

65-117; 67-651; 88-329;

## 597: CEDRENYL ACETATE

An ill-defined product consisting mainly of Cedryl acetate:



(Cedryl-): $C_{17}H_{28}O_2 = 264.41$
(Cedrenyl-): $C_{17}H_{26}O_2 = 262.40$

Colorless viscous oil. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol, miscible with most perfume oils.

Faint, fresh-woody odor of good tenacity, but without much character. There is considerable variation in the odor of materials from different suppliers (ester content, ratio of Cedrenyl/Cedryl- etc.).

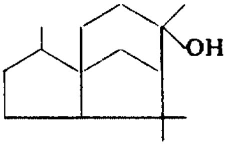
Used as a fixative in soap perfumes, household fragrances, mainly of the woody-piney types. Its actual "odor value" is insignificant.

Prod. by oxidation of Cedrene with Selenium dioxide in Acetic anhydride.

88-329;
see also CEDRYL ACETATE

## 598: CEDROL

"Cedarwood camphor".
Commercial "Cedrenol" consists largely of Cedrol.
See also: Cedrenol.



$C_{15}H_{26}O = 222.37$

White crystals. M.P. 86° C. Sp.Gr. 0.98.

Melting point of some qualities may be lower.

Lower grades of Cedrol are viscous liquids, usually with crystalline deposit.

Very faint odor (when pure, almost odorless) of Cedarwood type. A more "balsamic-sweet" odor is perceptible in low-grade Cedrols.

Used as a fixative for soaps, household product fragrances, detergent perfumes, industrial odors, etc.

However, the pure Cedrol is too expensive and yields too little odor to make it economically feasible in such fragrances.

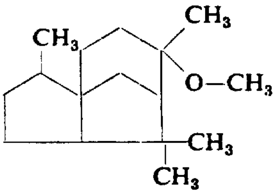
The actual volume used of Cedrol in perfumes as such is rather small.

Prod. by isolation from Virginia Cedarwood oil, followed by recrystallization.

4-29; 65-284; 67-676; 88-323; 106-89;

## 599: CEDROL METHYLETHER

Methyl cedryl ether.



$C_{16}H_{28}O = 236.40$

Colorless, slightly oily liquid. B.P. approximately 258° C.

Insoluble in water, soluble in alcohol and oils.

Refined-woody, pleasantly green odor of good tenacity.

This ether, occasionally offered commercially, may give refreshing and novel tonalities to woody and powdery fragrances, particularly those employing large amounts of Ionones, Labdanum, etc.

Its odor type is not exactly a rare one, and it tends to put rather narrow limits to the application of this ether. It will inevitably detract from the amount of sweetness already present in a composition, but it is stable and non-discoloring in soaps and powders, etc.

Overall, it is a material of little interest to the perfumer.

Prod.: by Methylation of Cedrol.

## 600: CEDRYL ACETATE

Structure: see CEDRENYL ACETATE

$C_{17}H_{28}O_2 = 264.41$

Ordinary commercial grade: White crystals, M.P. 40-42° C.
Refined grades: M.P. up to 80° C.

Sp.Gr. 1.05 (liquid).

Insoluble in water, soluble in alcohol, miscible in perfume oils.

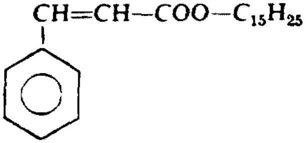
Woody, slightly leathery odor with a somewhat earthy undertone. It bears a slight similarity to Vetiver acetate in this respect.

Used as a fixative in perfumes, mostly soap perfumes of the woody type. It blends well with the Ionones, Lavandin oil, *iso*-Bornyl acetate, artificial musks, etc., but it contributes only little to the overall odor. It may form part of a leather complex but it will not lend much character to it.

Prod. by Acetylation of Cedrol.

4-29; 106-91; 33-502; 33-516;

## 601: CEDRYL CINNAMATE



$CH{=}CH{-}COO{-}C_{15}H_{25}$

$C_{24}H_{33}O_2 = 353.53$

Colorless viscous material, solidifying in the cold to a semi-crystalline mass.

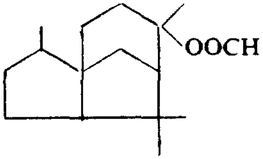
Insoluble in water, soluble in alcohol and oils.

Very faint, mainly woody odor with more sweetness than that of Cedrol, and with exceptional tenacity. The woody notes seem to dominate the terminal odors of this material, but this could be due to the fact that Cedryl cinnamate most likely appears commercially (when it appears at all) in a state of poor quality, probably containing large amounts of free Cedrol.

Since the acid portion of the molecule is practically odorless, chances are that the ester – if it is made available – will have an odor of Cedrol, and the author believes that there is no need for such an ester in perfumes.

The material can be considered practically obsolete.

## 602: CEDRYL FORMATE



$C_{16}H_{26}O_2 = 238.37$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol, miscible with oils.

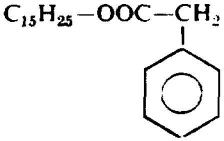
Mild, but persistent dry-woody odor. The woody notes are accompanied by a discrete amount of greenness, which completes an ensemble of some similarity to part of the Ambergris odor picture.

Recommended for use in perfume compositions, particularly in combination with Ionones, Rose bases, modern-aldehydic bases and in newer versions of "Men's fragrances", often in combination with Lime materials.

Undoubtedly cleaner than Cedryl acetate, the formate may have a place in the perfume laboratory of the modern and unconventional creative perfumer.

Sample: IFF-New York. (Nov. 1967).

## 603: CEDRYL PHENYLACETATE



$C_{15}H_{25}{-}OOC{-}CH_2$

$C_{23}H_{32}O_2 = 340.51$

Colorless viscous liquid. Insoluble in water, soluble in alcohol, miscible with perfume oils. B.P. 325° C. Sp.Gr. 1.03.

Very faint, woody-floral odor, somewhat reminiscent of the refined Methylionones. Extremely tenacious, but lends very little odor itself. With adequate blending into more volatile components, this ester may lend some interesting notes to the composition.

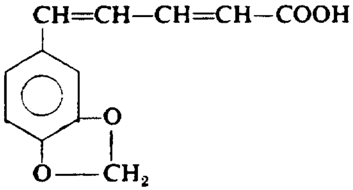
Blends excellently with Patchouli, Isoeugenol, Sandalwood, Cinnamic alcohol and cinnamates, etc. Very stable towards alkali and air (good in powders).

Prod. by esterification of Cedrol with Phenylacetyl chloride. (Direct esterification under azeotropic conditions is occasionally used on Cedrol plus Phenylacetic acid).

34-247; 34-248;

## 604: CHAVICINIC ACID

This is the
*alpha-cis-gamma-cis*-isomer of Piperic acid.
*3,4*-Methylenedioxy phenylpentadienoic acid.



$C_{12}H_{10}O_4 = 218.21$

White crystalline powder or crystal needles. M.P. 202° C.

Crystals darken upon exposure to daylight.

Practically odorless and tasteless, except for a distinct burning mouthfeel and pungency on mucous membranes.

Insoluble in water, soluble in alcohol and oils.

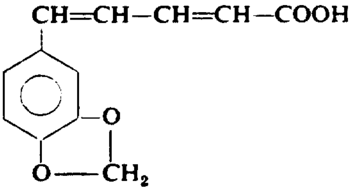
Used as part of the pungent principles in artificial Pepper and in spice blends.

Prod. from Heliotropine which is condensed with Acetaldehyde to *3,4*-Methylenedioxy cinnamic aldehyde. The latter is reacted with sodium acetate plus Acetic anhydride to yield Chavicinic acid and Piperic acid (the two stereo-isomeric components). All four possible stereoisomeric forms are known.

1-550; 68-780; 68-1016; 158-213; 1-857;

## 605: iso-CHAVICINIC ACID

This is the
*alpha-trans-gamma-cis*-isomer of
*5-(3':4'*-Methylenedioxyphenyl)-penta-*2:4*-dienoic acid.



$C_{12}H_{10}O_4 = 218.21$

White crystals, insoluble in water, soluble in alcohol and oils. M.P. 136° C.

Almost odorless. Burning-pungent mouthfeel and organoleptic effect but otherwise flavorless.

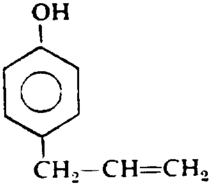
Used in artificial Black Pepper preparations and in spice blends.

Prod. from *trans-3,4*-Methylenedioxy cinnamylidene malonic acid with Quinoline.

1-857; 68-780; 68-1016; 158-213;

## 606: CHAVICOL

*para*-Allyl phenol.
*1*-Hydroxy-*4*-allyl benzol.



$C_9H_{10}O = 134.18$

Colorless liquid, solidifying in the cold.
M.P. 16° C. B.P. 236° C. Sp.Gr. 1.02.

Very slightly soluble in water, soluble in alcohol, miscible with oils.

Powerful, dry, tarry-medicinal "phenolic" odor, very penetrating and persistant.

Suggested for use in perfume compositions for "leather" or "smoke" effects, dry notes, etc. and – in the functional product – as an antiseptic.

Unstable under alkaline conditions, discolors in the presence of Iron and other metals in trace amounts.

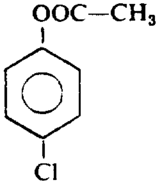
Prod. from Estragole (Methyl chavicol) by Grignard reaction with Ethyl Magnesium Bromide. Can also be isolated from Betel oil.

31-23; 65-505; 68-969; 72-43; 90-393; 100-230; 104-96;

## 607: para-CHLORO BENZYL ACETATE

(Commercial products contain considerable proportions of *ortho-* and *meta*-isomers).

*(para-)*



$C_8H_7ClO_2 = 170.60$

Colorless liquid. B.P. 250° C. Sp.Gr. 1.20.

Fruity, rather sharp, but clean odor of considerable tenacity. Overall type: Jasmin-Gardenia.

Suggested for use in perfume compositions. Probably a result of research in the field of chlorinated Benzyl esters, since Benzyl monochloroacetate has been recognized as a perfume chemical some decades ago. The subject ester is somewhat sharper than the Benzyl monochloroacetate, overall more powerful.

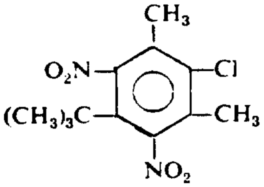
However, perfume materials with Chlorine atoms seem to scare perfumers generally, and these chemicals rarely attain true popularity.

Prod. by alkaline hydrolysis of *para*-Chloro benzylchloride followed by Acetylation of the alcohol.

4-30;

## 608: 2-CHLORO-4,6-DINITRO-1,3-DIMETHYL-5-tertiary-BUTYL BENZENE

One of the "original" Nitromusks, related to Musc Baur, and to Darzen's "Fluoride Musk".



$C_{12}H_{15}ClN_2O_4 = 286.83$

Pale yellowish crystals. Fairly soluble in alcohol, soluble in most perfume materials.

Odor similar to that of Musc Baur*), sweet, heavy, musky, slightly more pungent and less tenacious.

No longer of practical interest to the perfumer.

Produced from *para*-Cumene.

see also: 30-431; 31-196;

*) *2,4,6*-Trinitro-*3-tertiary*-butyl toluene (A. Baur, 1888).

## 609: CHLOROFORM

Trichloromethane.

$CHCl_3 = 119.39$

Colorless mobile liquid. Sp.Gr. 1.49. B.P. 61° C.

Diffusive, heavy, sweet-ethereal odor with considerable anaesthetic effect.

Soluble 0.8 % in water, miscible with alcohol and perfume oils.

May form poisonous Phosgene ($COCl_2$) when exposed to air and light.

Very sweet taste.

Although this chemical – to the author's knowledge – is no longer used in food flavor compositions, it has been included in this work partly because it has been used in flavors (Raspberry in particular), and still is used as a solvent in extracting certain botanicals for perfume and flavor use.

Old flavor formulations still show Chloroform as a sweetener in imitation fruit flavors.

Hazardous oral doses for human beings begin at about 0.2 grams or 0.13 ml. This amount could be present in 30 grams of toothpaste. The use of Chloroform as an initial flavor "burst" has been revived recently (1967) in several well-known dentifrice flavors.

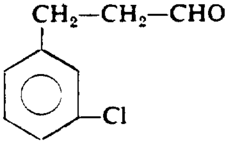
Prod.:

1) By reduction of Tetrachloromethane with Hydrogen.
2) From Acetone or Ethyl alcohol with Chlorine and Calcium hydroxide slurry.

7-113; 26-462; 100-243; B-I-61;

## 610: meta-CHLORO HYDROCINNAMIC ALDEHYDE

*3*-Chloro phenylpropionic aldehyde.



$C_9H_9ClO = 168.63$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 240° C.

Sweet, but rather pungent-floral odor of Hyacinth-type.

Moderate to poor tenacity.

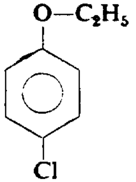
This rare aldehyde has been suggested for use in perfumery many decades ago, when Bromostyrol was still the fashionable and very frequently used carrier of Hyacinth-fragrances, but the modern tendency is directed away from halogenated aromatic compounds, although Bromostyrol is still used and highly appreciated by many perfumers.

The possible hazard of liberating Chlorine from a nucleo-halogenated chemical is very small, much less than the hazard of producing free Bromine from Bromostyrol. Yet there seems to be absolutely no interest in the title aldehyde, except for a few cases of "captive" use of this material.

Prod.: (several methods) e. g. by oxidation of *meta*-Chloro propylbenzene.

## 611: para-CHLORO PHENETHOLE

*para*-Chloro ethyl phenol.
*para*-Chloro ethoxy benzene.
*1*-Ethoxy-*4*-chlorobenzene.



$C_8H_9ClO = 156.62$

Colorless liquid. Solidifies in the cold.
M.P. 21° C. B.P. 212° C.

Very slightly soluble in water, soluble in alcohol and oils.

Phenolic-spicy odor, somewhat fruity, anisic-sweet, suggestive of Ylang-Ylang, Narcisse, Lily, etc.

In extreme dilution of this material one may find a lemony note.

Suggested for use in perfume compositions as a sweet-floral modifier.

However, its effects, toxicity, dermatological hazards, etc. remain to be investigated further.

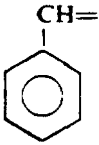
To the author's knowledge, this chemical is not used commonly in perfumes.

Prod. by Ethylation of *para*-Chloro phenol.

4-30; 26-460; B-VI-187; Dow Chem. Co., Aromatics Div. info. 1958.

## 612: omega-**CHLOROSTYROL**

*1*,$^2$-Chlorostyrol.
*omega*-Chlorostyrene.



$C_8H_7Cl = 138.60$

Colorless mobile liquid. B.P. 199° C.
Sp.Gr. 1.11.

Insoluble in water, soluble in alcohol and oils.

Penetrating, rather harsh-floral, Hyacinth-type odor, not as sweet as that of Bromostyrol.

Has been used in perfume compositions, mainly in inexpensive Hyacinth types as a modifier for Bromostyrol. However, there is a general tendency among perfumers to abandon the use of these and similar halogenated hydrocarbon chemicals on account of the possible hazard developing from traces of free halogen.

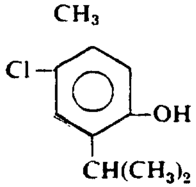
Very pure Chlorostyrol (and Bromostyrol) are actually useful and for special purposes excellent perfume chemicals, but they must be free from traces of free halogen, and they should not develop any trace of halogen upon storage of the perfume composition. Only under those circumstances would a continued use of these chemicals be justified.

Prod. from Chlorine plus Cinnamic acid in non-ionic solvent followed by boiling with aqueous Sodium carbonate. Another process uses Cinnamic acid and steam distils it with Calcium hypochlorite solution.

26-462; 31-200; 95-218; 96-194; B-V-476;

## 613: CHLOROTHYMOL

*6*-Chloro-*3*-oxy-*1*-methyl-*4*-*iso*-propyl benzene



$C_{10}H_{13}ClO = 184.67$

White (colorless) crystals. M.P. 62° C.

Almost insoluble in water, soluble in alcohol and oils. Thymol-like odor, but not as sweet, more "medicinal", less condiment-like.

However, the taste is definitely sweeter than that of Thymol. A 0.1% solution in water (saturated) has an odor very closely resembling that of Thymol.

This chemical finds more extensive use as a bactericidal additive than as a perfume chemical. It is included in this work because it occasionally appears in products related to the perfumer's or flavorist's work, and may interfere with his efforts to perfume or flavor the product.

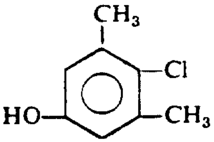
CHLORO CARVACROL finds similar use, but is, in the author's opinion, never used in perfumery.

Prod. by chlorination of Thymol in nonionic solvent with Sulfuryl chloride.

85-49; 100-248;

## 614: CHLOROXYLENOL

*para*-Chloro-*meta*-xylenol.
PCMX (abbreviated trade name).
*2*-Chloro-*meta*-*5*-xylenol.
*2*-Chloro-*5*-oxy-*1*,*3*-dimethylbenzol.
*4*-Chloro-*3*,*5*-dimethylphenol.



$C_8H_9ClO = 156.62$

Colorless crystals. M.P. 115° C.
B.P. 246° C.

0.03% soluble in water. Soluble in alcohol and oils.

Mild-phenolic type odor, rather dry but weaker than that of phenol or cresol.

Since this chemical is extensively used as a bactericide, and may occur in products related to the perfumer's or flavorist's work, it has been included in this book. To the author's knowledge, it is not used as such in perfume compositions.

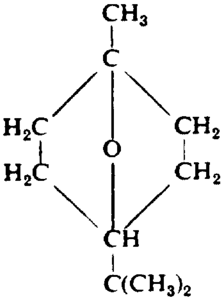
It is permitted as a disinfectant for exterior use where food (particularly meat) is handled, and in many other industries.

Prod. from *meta*-Xylenol by Chlorination with $Cl_2$ or $SO_2Cl_2$.

85-49; 100-249;

## 615: 1,4-CINEOLE

*1*,*4*-Epoxy-*para*-menthane.
(An isomer of Eucalyptol).



$C_{10}H_{18}O = 154.25$

Colorless mobile liquid. B.P. 173° C.
Sp.Gr. 0.90.

Almost insoluble in water, soluble in alcohol and oils.

Diffusive camphoraceous-fresh odor, more camphor-like, and not as sweet as Eucalyptol (see next monograph).

Cool, somewhat spicy-herbaceous taste.

Apart from the academic interest related to the olfactory similarity or dissimilarity of isomer chemicals, there is not much interest in this chemical. It is not nearly as readily available as its isomer, Eucalyptol.

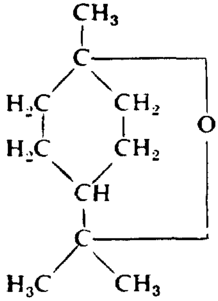
Prod.:

1) by dehydration of Terpin in the process of making Terpineol from Pinene.
2) by isolation from the red oil fractions of Camphor wood oil.

65-712; 90-678; 67-532;

# 616: 1,8-CINEOLE

Cineole.
Eucalyptol.
Cajeputol.
*1,8*-Epoxy-*para*-menthane.
*1,8*-Oxido-*para*-menthane.



$C_{10}H_{18}O$ = 154.25

One of the most widely distrubuted chemicals occurring in natural essential oils.
Colorless mobile liquid. B.P. 175° C.
Sp.Gr. 0.93. Solidifies in the cold, melts at +1° C.

0.6% soluble in ice-cold water, 0.4% soluble in water at room temperature. Soluble in Propylene glycol, miscible with alcohol and oils.

Fresh, diffusive, camphoraceous-cool odor of poor tenacity. Sweet and fresh, cool-camphoraceous taste and cool mothfeel unless very highly concentrated.

Widely used in perfume compositions for its refreshing effect in herbaceous type fragrances, Lavender, New Mown Hay, Fougère, etc. and in medicinal type odors for soap and household products. Also in masking odors for industrial purposes, unless Eucalyptus oil must be used for its lower cost.

This oxide has found increased usage during the 1965 66 period of abnormally high prices for Lavandin and Spike Lavender oils.

The odor of Eucalyptus is, in some countries, rated synonomous with masking odors for lavatories, etc., a fact which has an unquestionable psychological effect, causing people to reject the odor of Eucalyptus for oral-hygienic purposes, etc. Similar viewpoints has been observed about the use of Methylsalicylate in dentifrice in many European countries. Peculiarly enough, Methylsalicylate is still a popular candy-, soft-drink- and toothpaste flavor in the U.S.A., where the ester at the same time is used as a masking agent in toilet-bowl cleaners!

The "olfactory association" is quite human and common, but it may at times completely destroy the chances of a chemical from its use in flavors or other field.

Eucalyptol is extensively used in flavor compositions, particularly in all types of preparations for oral hygiejne, dentifrice, breath-sprays, mouthwashes, cough lozenges, pastilles, skin rubbing lotions, inhalator fluids, etc.

It seems, however, that its use in skin rubbing lotions has hampered its popularity as a candy flavor in the U.S.A.

Normal use concentrations are about 1 to 15 ppm in the finished (flavored) product, but concentrations as high as 200 ppm are found in chewing gpm.

G.R.A.S.*) F.E.M.A. No.2465.

Prod.: by isolation from "Eucapharma oils" (high-Cineole-Eucalyptus oils) e. g. the Eucalyptus globulus or E. Smithii.

Purification may be undertaken via the Resorcinol-adduct or the *ortho*-Cresol-adduct, both of whict are crystalline. Isolation by freezing is also used.

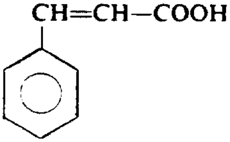
*1,8*-Cineole is one of the most inexpensive natural isolates (1968 approximately U.S. $ 2.10 pr. kilo) and the synthesis of this oxide has therefore no practical significance.

4-49; 26-552; 34-806; 65-708; 67-530; 77-138; 85-50; 100-439; 104-230; 160-924; B-XVII-24; 140-172;

*) Recent studies indicate that the hazard level is as low as 3 grams for adult human beings.

## 617: CINNAMIC ACID

*trans*-Cinnamic acid.
*trans-beta*-Phenylacrylic acid.
*trans-3*-Phenylpropenoic acid.
(*cis*-Cinnamic acid = Allo-cinnamic acid is known, but not included in this work).



$C_9H_8O_2 = 148.16$

White monoclinic crystals. M.P. 134° C. B.P. 300° C. Sp.Gr. (melted) = 1.06.

Soluble 0.04% in water, 24% in alcohol. Soluble in oils.

Very faint honeylike, balsamic odor, easily contaminated from outside odorants.

Finds very little use as such in perfumery.

Used in flavor compositions for imitation Cassia, spice blends, Cherry, Honey and various types of Cinnamon flavors, etc.

Concentration may reach 40 ppm in Ice cream.

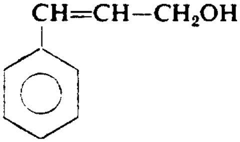
G.R.A.S. F.E.M.A. No.2288.

Prod.: (many methods) e. g.: Benzaldehyde plus Malonic ester with catalyst. Or: Benzaldehyde plus Acetic anhydride plus Sodium acetate (Perkin's reaction).

26-464; 34-582; 36-811; 68-995; 100-264; B-IX-572.

## 618: CINNAMIC ALCOHOL

Cinnamyl alcohol.
*3*-Phenyl-*2*-propen-*1*-ol.
Styryl carbinol.
*gamma*-Phenylallyl alcohol.
"Styrone".
Commercial products are chiefly *trans*-isomer, but perfumers are inclined to favor the uncommon *cis*-isomer for its finer odor.



$C_9H_{10}O = 134.18$

White or opaque solid crystalline mass. M.P. 32-33° C. B.P. 258° C. Sp.Gr. (liquid) 1.04.

Almost insoluble in water, soluble in alcohol, Propylene glycol, Glycerine, and most perfume and flavor oils, but practically insoluble in mineral oil.

Warm-balsamic, floral, sweet odor with a topnote of variable strength according to the purity of the material. Aldehyde content, which in good grades is well below 1.0 may in other commercial lots be about 1.5 and this will influence the odor of the alcohol perceptibly.

Overall Hyacinth-type odor with some resemblance to Rose. Widely used in perfume compositions, including many low-cost floral fragrances, soap perfumes, etc. Blends excellently with Amylsalicylate, Phenylethylalcohol, aromatic propionates, benzoates, etc. Generally as a modifier-blender with fair tenacity and moderate fixative value.

Used in flavor compositions for imitation Apricot, Brandy, Cinnamon, Grape, Liquor, Peach, Plum, Prune, Nut, Raspberry, Spice, Strawberry, Black Walnut, etc.

Concentration is about 35 ppm. in baked goods, but may run as high as 700 ppm. in chewing gum.

G.R.A.S. F.E.M.A. No.2294.

F.C.C. 1964-805.

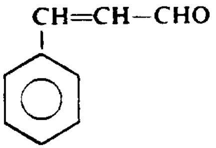
Prod.:

1) By reduction of Cinnamic aldehyde (yields *trans*-isomer).
2) By reduction of Phenylpropargyl aldehyde dimethylacetal (yields *cis*-isomer).

26-464; 34-582; 36-815; 68-981; 77-176; 100-264; 106-96; B-VI-470;

## 619: CINNAMIC ALDEHYDE

*trans*-Cinnamaldehyde.
Cinnamal.
3-Phenylpropenal.
*gamma*-Phenylacrolein.
"Cassia aldehyde".



$C_9H_8O = 132.16$

Yellow liquid. Sp.Gr. 1.11. B.P. 252° C.

Solidifies in the cold, melts at minus 7° C.

Almost insoluble in water, almost insoluble in common hydrocarbon solvents, miscible with alcohol and most perfume and flavor oils.

Oxidizes easily in air, resinifies under UV-light. Volatile with steam.

Warm-spicy-balsamic odor, suggestive of Cassia-cinnamon. Good tenacity and lasting sweetness.

Sweet and warm-spicy taste with little or no pungency at normal use level.

Used in perfumery as a sweetener and powerful spicy ingredient in low-cost fragrances mainly for household products, in masking odors and in detergents and soaps where discoloration is not visible (Cinnamic aldehyde will discolor white soaps). Trace amounts are used as a warm-spicy and sweet note in floral-balsamic fragrance types, heavy florals and oriental fragrance types. It introduces interesting notes when used discretely in Rose, Hyacinth or in woody fragrances, etc.

Extensively used in flavor compositions. Part of the classic "Sen-Sen" flavor, it has later entered mouth-wash, dentifrice and candy flavors in the shape of many different flavor types; Spice, Cinnamon, Cola, Mint, etc. and it forms a minor component of many Apple, Cherry, Cream Soda, Liquor, Nut, Pecan, Vanilla, etc. for soft drinks, candy, chewing gum, etc.

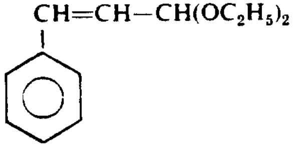
Concentration may be about 700 ppm. in candy, and up to 5000 ppm. in chewing gum. Certain types of chewing gum flavor consist almost entirely of Cinnamic aldehyde.

G.R.A.S. F.E.M.A. No.2286.

Prod. by condensation of Benzaldehyde with Acetaldehyde (alkali condens.).

7-103; 31-61; 68-984; 77-19; 77-20; 77-205; 100-263; 26-464; B-VII-8; 106-98;

## 620: CINNAMIC ALDEHYDE DIETHYL ACETAL



$C_{13}H_{18}O_2 = 206.29$

Almost colorless oily liquid. B.P. 251° C. (very close to that of Cinnamic aldehyde). Sp.Gr. 0.98.

Practically insoluble in water, soluble in alcohol and oils.

Faint, but fresh-green, slightly spicy, oily-sweet odor. Taste is mild and oily-sweet, not nearly as sweet as the aldehyde.

Used occasionally in perfume formulations as a modifier and "new" note in modern-aldehydic or spicy-fruity fragrance types.

Stable in soap, but does not contribute much "spice" odor and can not be considered a suitable substitute for the aldehyde.

Since this acetal – like most other acetals – is unstable under mildly acid conditions, it finds little, if any, use in flavor compositions.

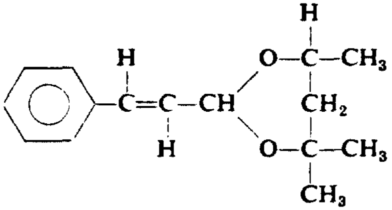
Prod.:

1) From Cinnamic aldehyde and Formiminoethylether hydrochloride.
2) From Cinnamic aldehyde and Ethanol with dry HCl gas.

5-315; 86-135; 37-282;

## 621: CINNAMIC ALDEHYDE-2,4-DIHYDROXY-4-METHYLPENTANE ACETAL

*2*-Styryl-*4,4,6*-trimethyl-*1,3*-dioxan.
A cyclic acetal.



$C_{15}H_{20}O_2 = 232.33$

Almost colorless, slightly viscous liquid.
B.P. approximately 285° C.

Practically insoluble in water, soluble in alcohol, Propylene glycol and most perfume and flavor oils.

Soft, tenacious, natural Cinnamon-type odor, not nearly as harsh as Cinnamic aldehyde, yet rich and lasting as the aldehyde itself.

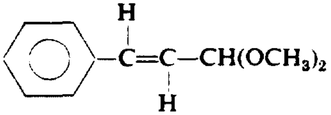
Has been suggested for use in place of Cinnamic aldehyde where the alkali-instability of the aldehyde is a disadvantage. However, the cost of the Acetal – as long as it is not widely used and demanded – is prohibitive for use as a substitute except in the few cases of higher cost fragrances. The main outlet for Cinnamic aldehyde is the low-cost fragrance type.

Prod. from Cinnamic aldehyde by condensation with *2*-Methylpentane-*2,4*-diol.

31-73;

## 622: CINNAMIC ALDEHYDE DIMETHYL ACETAL

Cinnamal dimethylacetal (*trans-*).



$C_{11}H_{14}O_2 = 178.23$

Almost colorless oily liquid. B.P. 239° C.
Sp.Gr. 1.02.

Fresh-green, spicy-herbaceous Cassia-cinnamon type odor, more Cassia-like than the Diethyl acetal, yet less harsh than the aldehyde.

Sweet spicy-herbaceous taste, but not nearly as sweet as the aldehyde.

Used as a lasting topnote ingredient in many types of "modern" fragrances, not only in copies of successful French perfumes, but also in general as a novelty along with aldehydic-floral or Oriental-spicy or sweet-woody fragrance types. It forms interesting topnotes with alifatic aldehydes in Rose-Jasmin fragrances, and gives pleasant variations of woody-Oakmoss types.

Stable in soap and may introduce Cinnamon type odor when used at a sufficiently high level of concentration.

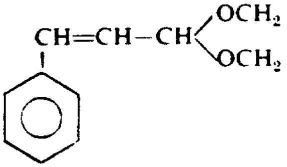
Prod.: By condensation of Cinnamic aldehyde with Methanol.

NOTE: It should be noted that pure, aldehyde-free acetal is practically colorless and carries little or no odor similarity to the aldehyde. Commercial lots often contain 2-4-6 percent free aldehyde, sometimes even requested by the customer, perhaps as a carry-over from times when the acetal could not be produced aldehyde-free.

5-315; 37-282; 68-984; 86-135;

## 623: CINNAMICALDEHYDE ETHYLENE GLYCOL ACETAL

"Cinncloval".
*2*-Styryl-*1,3*-dioxolane.



$C_{11}H_{12}O_2 = 176.22$

Almost colorless oily liquid.
B.P. approximately 265° C.

Insoluble in water, soluble in alcohol and oils.

Pleasant, soft-spicy, warm, sweet odor suggestive of Cinnamon, rather than of Cassia (a softness resembling that of Clove). Not nearly as harsh as the odor of the aldehyde.

Sweet-spicy Cinnamon-Allspice taste, but not quite as sweet as the aldehyde.

This acetal is used in flavor compositions such as Allspice, Cassia, Cinnamon, Clove and various Spice blends, etc.

Concentration is usually very small (a few ppm.) in the finished product.

Under distinctly acid conditions (pickles, etc.) the acetal will decompose and act as Cinnamic aldehyde. This will change the flavor effect of the composition. However, this acetal is moderately stable under mildly acid conditions.

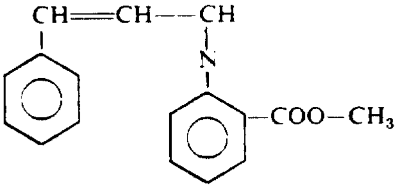
Prod.: From Cinnamic aldehyde and Ethylene glycol by condensation.

G.R.A.S. F.E.M.A. No.2287.

31-73;

## 624: CINNAMIC ALDEHYDE-METHYLANTHRANILATE

(A type of "Shiff's base").



$C_{17}H_{15}NO_2 = 265.32$

Intensely yellow, viscous liquid. Darkens further with age.

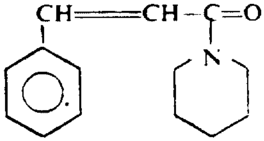
This product has only little more than academic interest. The spicy cinnamic note is rarely wanted along with Orangeblossom-notes, except in certain variations of the Oriental fragrances.

The two odor types can be obtained with less hazard of discoloration if the Methyl-*N*-methylanthranilate is used plus e. g. Methylcinnamic aldehyde, both more stable components, not forming any sort of condensation product.

Prod. by "condensation" of equal Mols. of Cinnamic aldehyde and Methyl anthranilate.

## 625: 1-CINNAMOYL PIPERIDINE

*N*-Cinnamoyl piperidine.



$C_{14}H_{17}NO = 215.30$

White crystals, M.P. 123° C.

Practically insoluble in water, soluble in alcohol and most oils.

Virtually odorless, and not volatile with steam.

Although this chemical has no taste, basically speaking, it produces an intensely burning mouthfeel, sometimes called a "bite", typical of certain purely pungent principles.

It was identified more than 20 years ago as one of the pungent principles of Pepper, and a synthesis has been developed to make the chemical commercially available.

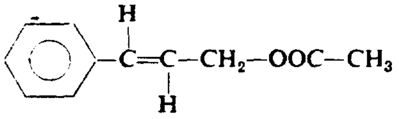
Prod.: from Cinnamoyl chloride and Piperidine.

Litt.:
1) Arthur D. Little: in Food Technology, 1956, Vol. X, No. 9, pp. 423-427.
2) Journal of American Chemical Society, 67, 903 (1945).

see also: 1-528;

## 626: CINNAMYL ACETATE

*trans-gamma*-Phenylallyl acetate.



$C_{11}H_{12}O_2$ = 176.22

Colorless oily liquid. B.P. 262° C.
Sp.Gr. 1.05.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet, mild-balsamic and slightly floral-fruity odor. The spicy note has a tendency of "showing through" and disturb the fragrance picture of a composition, often more than what is desirable. In this respect, it is the most "cinnamic" of all the esters, more than the Formate and more than the Propionate, etc.

Used as a modifier for Cinnamic alcohol and as a warm-spicy-floral note in heavy florals, Hyacinth, etc. It can also introduce warmth to a Rose composition at a discrete level of concentration.

Used in flavor compositions for imitation Apple, Apricot, Berry, Cherry, Cinnamon, Cassia, Grape, Peach, Pineapple, Quince, Vanilla, etc.

Concentration is generally low – about 12 to 18 ppm. in the finished product.

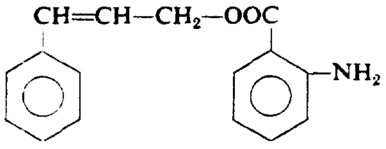
Prod. by direct esterification of Cinnamic alcohol with Acetic acid (or anhydride) under azeotropic conditions with or without a catalyst.

G.R.A.S. F.E.M.A. No.2293.

5-60; 34-461; 90-338; 106-99; 140-137;

## 627: CINNAMYL ANTHRANILATE

Cinnamyl-*ortho*-aminobenzoate.



$C_{16}H_{15}NO_2$ = 253.30

White crystalline powder when pure. Greyish-ambercolored crystalline mass (some commercial products). M.P. 64° C. B.P. 332° C. Sp.Gr. (liquid) 1.18.

Insoluble in water, soluble in alcohol and perfume oils, almost insoluble in Propylene glycol.

Mild, but extremely tenacious fruity-floral odor, mostly Rosy-floral, almost Magnolia-like.

Some commercial grades have pronounced "Anthranilate"-type odor, harsh-Orangeblossom, depending upon the method by which the ester has been produced.

Occasionally used in perfumes as a fixative in Orangeblossom, Honeysuckle, Hyacinth or other heavy floral notes.

Used in flavor compositions for imitation Grape, Cherry, Honey, Vanilla, etc.

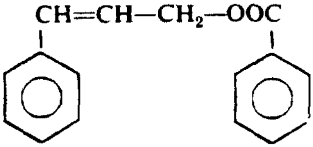
The concentration in gelatinous desserts may be about 30 ppm, while it can be up to 750 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2295.

Prod. from Isatoic anhydride plus Cinnamic alcohol.

34-1011; 34-1012; 106-100;

## 628: CINNAMYL BENZOATE



$C_{16}H_{14}O_2 = 238.29$

White crystalline powder. M.P. 31° C. B.P. 335° C. Sp.Gr. 1.04 (liquid).

Insoluble in water, soluble in alcohol and oils.

Mild-spicy, tenacious and balsamic odor. Freshly prepared and pure grade materials are odorless to many people, faintly "musky" to others.

Used as a fixative for Oriental fragrance types, heavy florals such as Hyacinth, but in general, this ester is too expensive for such purpose, since good fixation requires a considerable amount of crystalline material (up to 10 percent or more), and a similar fixation can be achieved with less expensive crystalline fixatives.

Used in flavor compositions for imitation Butter, Caramel, Raspberry and in a multitude of Fruit flavors.

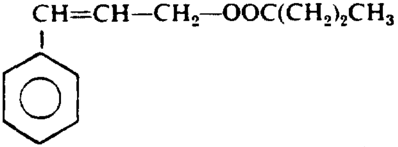
Concentration is usually up to 15-18 ppm in candy.

Prod. from Cinnamyl chloride plus Sodium benzoate.
or: from Cinnamic alcohol and Benzoic acid by azeotropic process.

4-31; 5-60; 34-463; 86-31;

## 629: CINNAMYL BUTYRATE

Phenyl propenyl-*n*-butyrate.



$C_{13}H_{16}O_2 = 204.27$

Colorless liquid. Sp.Gr. 1.02. B.P. 300° C.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-balsamic, rather faint, but actually heavy odor, resembling Phenylethyl butyrate, but less floral. The undertone is floral and rich, but the overall impression is fruity-balsamic.

Useful in Sweet Pea, Muguet, Rose, Tuberose, and as a fixative in Citrus fragrances. Blends well with Labdanum, Styrax, Benzoin, Citronellol, Geraniol, Ionones, etc.

Occasionally used in flavor compositions for imitation Orange, Citrus and Fruit (Tutti-frutti) flavors.

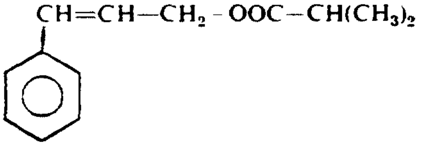
Concentration is usually mere traces (a few ppm) in the finished product.

G.R.A.S. F.E.M.A. No.2296.

Prod. by direct esterification of Cinnamic alcohol with *n*-Butyric acid under azeotropic conditions.

4-31; 33-734; 86-31; 100-101;

## 630: CINNAMYL-iso-BUTYRATE



$C_{13}H_{16}O_2 = 204.27$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol. Sp.Gr. 1.01. B.P. 254° C.

Fresh-fruity, mild-balsamic very sweet odor somewhat reminiscent of ripe Banana with an added fragrance of Plum.

Sweet, balsamic-fruity taste with a "deep" aroma of "preserved" fruit type.

Occasionally used in perfumes, e.g. fragrances for lipsticks, and in floral bases such as Mimosa, Cassie, Magnolia. It is useful in Oriental fragrance types and blends excellently with Patchouli and sweet-woody fragrance materials. Its tenacity is very good and the stability satisfactory.

Used in flavor compositions for imitation Apple, Banana, Citrus, Nut, Walnut, Grape, Peach, Pear, Pineapple, Strawberry, etc.

Concentration is mostly at the level of a few ppm in the finished product, but it will often be as high as 150 ppm in chewing gum.

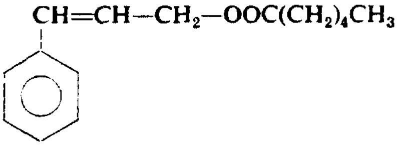
G.R.A.S. F.E.M.A. No.2297.

Prod. by direct esterification of Cinnamic alcohol with *iso*-Butyric acid under azeotropic conditions.

77-186; 86-31; 106-103; 155-94; 140-140;

## 631: CINNAMYL CAPROATE

Cinnamyl hexoate.



$C_6H_5$–$CH{=}CH{-}CH_2{-}OOC(CH_2)_4CH_3$

$C_{15}H_{20}O_2 = 232.33$

Colorless, slightly oily liquid. B.P. 290° C. Sp.Gr. 1.01.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Fruity-green, slightly spicy, sweet and warm odor, remotely reminiscent of Banana and Mango.

Sweet, deep-fruity, somewhat "dry" taste with a mild-spicy undertone.

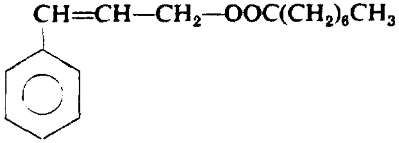
Rarely used in perfumery, occasionally used in flavor compositions as a modifier for heavy-fruity compositions, not only Banana, but Plum, Pineapple, etc. and certain types of "Polynesian-fruit blends".

Prod. by direct esterification of Cinnamic alcohol with Caproic acid under azeotropic conditions.

34-463; 34-1230; 86-31;

## 632: CINNAMYL CAPRYLATE

Cinnamyl octoate.



$C_6H_5$–$CH{=}CH{-}CH_2{-}OOC(CH_2)_6CH_3$

$C_{17}H_{24}O_2 = 260.38$

Colorless, somewhat viscous liquid. B.P. 345° C. Sp.Gr. 1.00.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Very mild, balsamic-winey odor, slightly oily-fruity, (nondescript fruity).

Very mild, sweet-balsamic-fruity taste. However, the taste is perceptible at quite high dilutions (beyond 1-500,000).

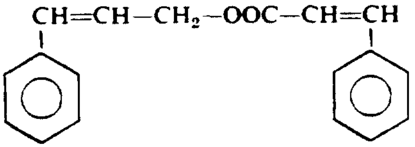
This ester is rarely used in perfumes and flavors. Occasionally as a modifier for the lower esters of Cinnamic alcohol, or as a fixative for those.

Prod. by direct esterification of Cinnamic alcohol with Caprylic acid under azeotropic conditions.

34-463; 35-404;

## 633: CINNAMYL CINNAMATE

"Styracine".
Phenylallyl cinnamate.



$C_{18}H_{16}O_2 = 264.33$

White or colorless crystals. M.P. 45° C. B.P. 370° C. Sp.Gr. (liquid) 1.16.

Insoluble in water and Propylene glycol. 4% soluble in alcohol, soluble in most perfume oils.

Very mild, but very tenacious balsamic-floral, soft odor. Hardly any spice note at all.

Useful as a fixative in heavy florals, exotic florals, Carnation type fragrances, Hyacinth, Tuberose, etc. and in smaller amounts in Magnolia and similar fragrance types. It blends also well with Labdanum, Patchouli and Oakmoss.

Traces of this ester are used in flavor compositions mostly as a fixative in fruity types.

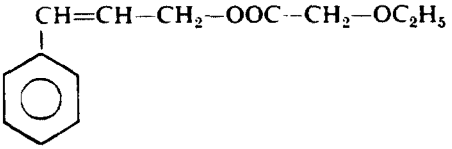
G.R.A.S. F.E.M.A. No.2298.

Prod. from Cinnamic aldehyde plus Aluminum ethylate in Ether. (Can also be produced by azeotropic type process from the alcohol and the acid).

4-31; 34-263; 86-31; 90-350; 95-186; 96-213; 156-86;

## 634: CINNAMYL ETHOXYACETATE

Glycolic ethyl ether, cinnamylester.



$C_{13}H_{16}O_3 = 220.27$

Colorless viscous liquid.

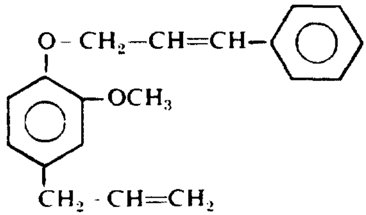
Has been reported as a chemical with possible interest to the perfumer. A great number of Ethoxy acetates, Methoxy acetates, etc. have been produced in perfumery research, but only a few of these chemicals have remained on the perfumer's shelf as standard items.

This ester is, to the author's knowledge, very rarely used in perfumes or flavors.

Prod.: from Cinnamic alcohol and Ethoxyacetic acid.

## 635: CINNAMYL EUGENOL

*Eugenol cinnamyl ether.*



$C_{19}H_{20}O_2 = 280.37$

White or creamy-white crystals or crystalline mass. B.P. 292° C. Sp.Gr. 1.01 (liquid).

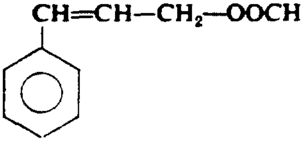
Very mild, spicy-balsamic odor. It is claimed that when this chemical is absolutely pure, it has no perceptible odor. Most conceivably, the rare commercial lots have a surplus of one component or trace impurities which sharply influence the odor of the ether.

Could find some use as a fixative, but can probably not compete with the common, lower-cost fixatives of related chemical composition and similar odor type and fixative effect.

Prod. from Eugenol sodium plus Cinnamyl chloride.

34-1115; 86-31;

## 636: CINNAMYL FORMATE



$C_{10}H_{10}O_2 = 162.19$

Colorless, slightly oily liquid. B.P. 250° C. Sp.Gr. 1.08.

Insoluble in water, soluble in alcohol and oils.

Green-herbaceous, yet "cinnamic" odor, balsamic, but more "dry"-fruity than the higher cinnamates. Powerful and of good tenacity.

An interesting item in perfume compositions. Blends excellently with Patchouli and "heavy" woody materials, good effects in Chypre and Oriental fragrance types. Very good stability under normal conditions in functional products.

Used in trace amounts in flavor compositions, particularly Apple, Banana, Cherry, Pear, Spice, etc.

It is particularly interesting in imitation Banana, where it can produce true-to-Nature notes if used discretely, and perhaps in combination with Mimosa absolute, also in traces.

G.R.A.S. F.E.M.A. No.2299.

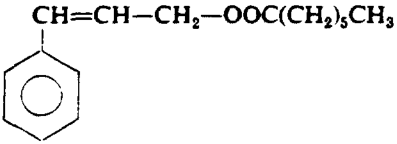
Prod.

1) from Cinnamic alcohol plus Carbon monoxide under pressure.
2) from Cinnamic alcohol, Acetic anhydride and Formic acid.

4-31; 34-463; 86-31; 106-102; 140-133;

## 637: CINNAMYL HEPTOATE

Cinnamyl heptylate.



$C_{16}H_{22}O_2 = 246.35$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 330° C. Sp.Gr. 0.99.

Sappy-green, slightly woody-earthy, but overall sweet floral-balsamic, slightly fruity odor, reminiscent of Hyacinth-foliage or Iris-foliage.

Although a relatively rare item, this ester is interesting for certain applications in perfumery. It forms for instance an intermediate or "liaison" between the dry-green notes of Galbanum, and the heavy-sweet notes of an Ionone-Patchouli base, a theme not uncommon in perfumery. Apart from giving "life" to a Hyacinth, it may give freshness to many fragrances rich in Ionones which tend to produce heavy notes.

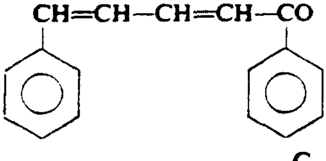
The ester finds, to the author's knowledge little, if any, application in flavors.

Prod. by direct esterification of Cinnamic alcohol with Heptanoic acid under azeotropic conditions.

34-462; 35-59; 86-31;

## 638: CINNAMYLIDENE ACETOPHENONE

*1,5*-Diphenyl-*1,3*-pentadien-*5*-one.



$C_{17}H_{14}O = 234.30$

Pale yellowish crystals. M.P. 103° C.

Insoluble in water, poorly soluble in Propylene glycol. Soluble in alcohol and oils.

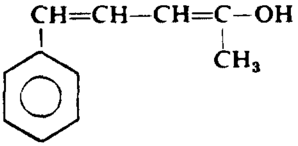
Intensely sweet, but somewhat pungent-floral-herbaceous odor of considerable tenacity.

Has been suggested for use in perfume compositions, but it is most likely that its color and possible skin irritation hazard (compare related chemicals) has prevented this material from becoming a popular perfume item.

Prod. by condensation of Cinnamic aldehyde with Acetophenone under alkaline conditions.

68-1183;

## 639: CINNAMYLIDENE METHYLCARBINOL



$C_{11}H_{12}O = 160.22$

Colorless to pale yellowish, viscous liquid.

Tenacious-floral, balsamic-green odor.

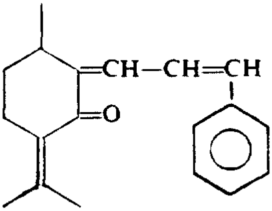
Has been suggested for use as a fixative for delicate floral fragrances, Lilac, Appleblossom (which unfortunately often is "created" as a vulgar, pungent, harsh fragrance!), Sweet Pea, Magnolia, etc.

The material is very rarely offered under its proper chemical name, and has apparently not achieved much popularity. It is most conceivable that its rather high cost is prohibitive for its more extensive use.

4-13; 31-23;
See also:
Homocinnamyl alcohol, sometimes called:
Methyl cinnamylidene carbinol (confusing).

## 640: CINNAMYLIDENE PULEGONE

Cinnamal pulegone.
*1*-Methyl-*2*-cinnamylidene-*4*-*iso*-propylidene cyclohexan-*3*-one.



$C_{19}H_{22}O = 266.39$

Yellowish oily liquid, solidifying in the cold.

Very slightly soluble in water, soluble in alcohol and oils.

Intensely sweet, honey-like, tenacious odor with herbaceous-tobacco-like undertone.

The title material is used in perfume compositions as supporting note in floral bases, but the material is not offered commercially under its proper chemical name, although this type of ketone has been suggested since 1930. As a separate perfume chemical, it has never achieved much fame, but it has its circle of enthousiasts among perfumers who are familiar with its virtues and drawbacks.

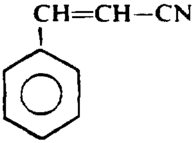
Its keeping qualities are not very good, and it tends to acquire a yellowish color on exposure to air and daylight.

Prod.: by condensation of Pulegone with Cinnamic aldehyde under mildly alkaline conditions.

3-208;
See also: Anisylidene thujone.

## 641: CINNAMYL NITRILE

Styryl cyanide.
"Cinnamalva" (I.F.F.).
The name "Cinnamyl nitrile" is often used commercially, but is incorrect.



$C_9H_7N = 129.16$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful, warm-spicy, oily and slightly floral odor of moderate to poor tenacity. The spicy note is very Cinnamon-like, but lacks the natural dry notes of the Cinnamon bark. The oily character is by no means a disadvantage, since it makes the material more versatile than Cinnamon bark oil and Cinnamic aldehyde.

The terminal notes, which appear rather quickly on a perfume blotter, show the typical "Nitrile-character" which, however, blends very pleasantly with the Styrene notes.

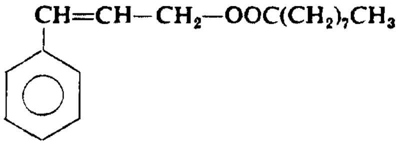
This material, a member of a long series of Nitriles developed to (hopefully) substitute for unstable aldehydes,'is a comparatively new item on the perfumer's shelf. It blends very well with the Rose materials, Hyacinth and Styrax, and it supports spicy notes in complexes with Clove or Eugenol. It gives interesting effects in Fir needle fragrances (room sprays etc.), and will, with adequate companions, partly substitute for Cinnamic aldehyde in many cases.

Prod.: (several methods) e.g. from Styryl bromide and Potassium cyanide.

NOTE: The nitrile is stable under mildly alkaline conditions (soaps and detergents), but decomposes under acid conditions (most flavored products).

## 642: CINNAMYL PELARGONATE

Cinnamyl nonanoate.



$C_{18}H_{26}O_2 = 274.41$

B.P. 340° C. Sp.Gr. 0.98.

Colorless, viscous liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

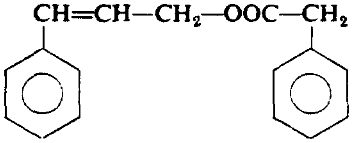
Faint, but sweet and fruity-oily odor of somewhat orrisy type and excellent tenacity.

Occasionally used in perfumery as a modifier or fixative for delicate florals, Lilac, Sweet Pea, Magnolia, etc., or as a new note in Oriental fragrance types. Its influence upon the odor of Patchouli oil is quite pleasant and interesting, and it seems to amplify the Ionone effect of a fragrance using these chemicals.

Prod. by direct esterification of Cinnamic alcohol with Nonoic acid under azeotropic conditions.

4-31; (see also American Perfumer 1948, page 123).

## 643: CINNAMYL PHENYLACETATE



$C_{17}H_{16}O_2 = 252.32$

Colorless, slightly viscous liquid. Insoluble in water, soluble in alcohol and oils.

B.P. 333° C. Sp.Gr. 1.09.

Mild, but deep and sweet, Tolubalsam-like odor with herbaceous-floral undertones and outstanding tenacity.

Occasionally used in perfume compositions, mainly in Oriental fragrance types. This chemical forms an excellent intermediate and link between Patchouli and Civet notes, combining these notes into a more delicate and pleasant unity.

Traces of this ester are used in flavor compositions, mainly for Chocolate, Honey and Spice compositions.

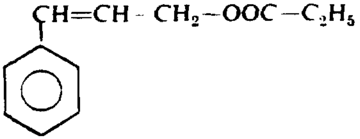
G.R.A.S. F.E.M.A. No.2300.

Prod. from Cinnamyl chloride and Sodium phenylacetate. It is possible to prepare the ester by the conventional method (azeotropic esterification).

34-246; 86-31;

## 644: CINNAMYL PROPIONATE

*gamma*-Phenylallyl propionate.
3-Phenyl-2-propenyl propanoate.



$C_{12}H_{14}O_2 = 190.24$

Colorless, slightly oily liquid. B.P. 289° C. Sp.Gr. 1.03.

Almost insoluble in water, soluble in alcohol, miscible with most perfume oils.

Fruity-balsamic, but also floral (rather rosy) odor with mild cinnamon-like undertone.

Sweet, warm, fruity-spicy taste of considerable power.

Occasionally used in perfume compositions, mostly in Oriental fragrance types as a modifier for the more pronounced, spicy items. It blends with Oakmoss into a very pleasant composition, particularly in the presence of Clove bud and Patchouli oils, or Bay leaf oil, etc.

Used in flavor compositions for imitation Apple, Berry, Chocolate, Currant, Grape, Peach, Pear, Pineapple.

Concentration in the finished product is usually only a few ppm (traces), but may in chewing gum reach 50 ppm.

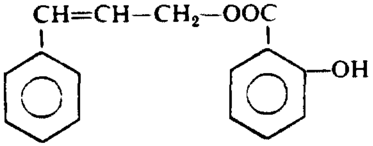
Prod. by direct esterification of Cinnamic alcohol with Propionic acid (or Propionic anhydride) under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2301.

33-620; 34-463; 86-31;

## 645: CINNAMYL SALICYLATE

Cinnamyl-*ortho*-hydroxybenzoate.



$C_{16}H_{14}O_3 = 254.29$

White crystals.

Insoluble in water, soluble in alcohol, miscible with most perfume oils.

Very faint, sweet and pleasant balsamic odor. A trace of a rosy or nondescript-floral undertone. Good tenacity.

This chemical is very rarely offered from the usual suppliers or manufacturers of perfume chemicals, and it is not a common item on the perfumers' shelves.

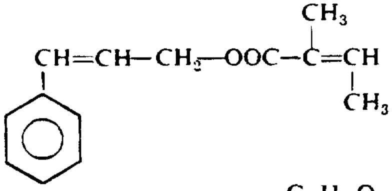
It carries the same drawback as most other Salicylates, sensitivity to alkali and iron, and this contributes to its poor future as a perfume chemical.

Prod. by azeotropic esterification of Cinnamic alcohol and Salicylic acid. Also from Cinnamyl chloride and Sodium salicylate.

34-788; 86-32;

## 646: CINNAMYL TIGLATE

Cinnamyl-*trans-alpha*-methylcrotonate.
Cinnamyl-*trans-alpha-beta*-dimethylacrylate.



$C_{14}H_{16}O_2 = 216.28$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very pleasant, floral-herbaceous odor, suggestive of Styrax and Peru balsams, or rather of the distillates of same. A faint, green note is perceptible in the undertones. Good tenacity.

Suggested for use in perfume and flavor compositions. This ester is of comparatively recent date, and does not appear on the G.R.A.S. list yet, but it would be an interesting item in minty dentifrice flavors. Its taste is pleasant, sweet and warm, quite powerful.

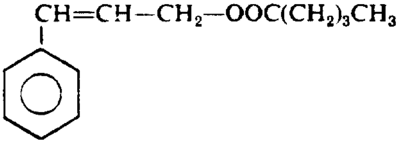
In perfume compositions this ester could find use as a new note in "Leather" fragrance types, as a modifier for pyrogenated Styrax, and as a good, pleasant smelling fixative for the citrusy notes usually present.

Prod. by direct esterification of Cinnamic alcohol with Tiglic acid under azeotropic conditions.

(Fritzsche Bros. sample and info.).

## 647: CINNAMYL VALERATE

Cinnamyl-*n*-pentanoate.



$CH{=}CH{-}CH_2{-}OOC(CH_2)_3CH_3$

$C_{14}H_{18}O_2 = 218.30$

Colorless liquid.

Delicately floral, rather rosy odor of good tenacity and with a trace of fresh-green, herbal tone.

Could find use in perfumery as a modifier or variant in rose compositions.

However, the *n*-valerate is a rather uncommon ester, while the *iso*-valerate is the ester most often referred to, even when the name is quoted as "Cinnamyl valerate".

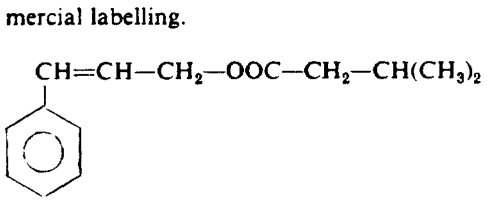
See next monograph.

Prod. by direct esterification of Cinnamic alcohol with *n*-Valeric acid under azeotropic conditions.

86-32;

## 648: CINNAMYL-iso-VALERATE

Often called "Cinnamyl valerate" in commercial labelling.



$CH{=}CH{-}CH_2{-}OOC{-}CH_2{-}CH(CH_3)_2$

$C_{14}H_{18}O_2 = 218.30$

Colorless liquid. B.P. 313° C. Sp.Gr. 1.00.

Insoluble in water, soluble in alcohol, miscible with most perfume oils. Poorly soluble in Propylene glycol.

Fresh, but delicately floral, rosy odor. Balsamic, almost sweet-tobacco-like undertones. Good tenacity.

Interesting in perfume compositions of the light floral type, Peony, Magnolia, Sweet Pea, Freesia, and in Rose variations.

Used quite frequently in flavor compositions for imitation Apple, Apricot, Cherry, Chocolate, Grape, Maple, Nut, Peach, Pineapple, Plum, Spice, Strawberry, etc. Also in tobacco flavorings.

Concentration is most often only a few ppm in the finished product, but may reach 40 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2302.

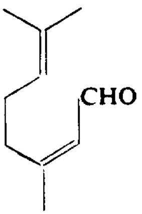
Prod. by direct esterification of Cinnamic alcohol with *iso*-Valeric acid under azeotropic conditions.

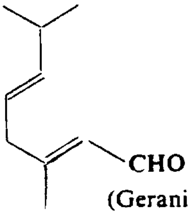
4-31; 33-934; 86-31;

## 649: CITRAL

Geranial (*trans-alpha*-Citral).
Neral (*cis* = *beta*-Citral).
"Lemarome" (Hoffmann-laRoche).
*3*,*7*-Dimethyl-*2*,*6*-octadienal.

Neral:





(Geranial)

$C_{10}H_{16}O = 152.24$

Colorless liquid. Sp.Gr. 0.89. B.P. 228° C (under slight decomposition). May turn yellowish when exposed to air and daylight.

Insoluble in water, soluble in alcohol, miscible with most perfume and flavor oils.

Widely used as a powerful Lemon-fragrance chemical, but suffers from poor stability in many types of functional products. Air, alkali and daylight have a deteriorating influence upon this aldehyde, and Anthranilates, Indole, Quinolines and many other perfume chemicals form dark colored reaction products with Citral. Accordingly, its use is somewhat restricted and there is a low limit of concentration of Citral for most perfumes.

Olfactory research during the past few decades has confirmed that Nitriles often have odors similar to those of the corresponding Aldehydes, and this is how Geranyl nitrile (see that monograph) has become increasingly popular in perfume compositions.

Very commonly used in flavor compositions. High dilution of the aldehyde in the functional product, usually low $p_H$ of the product, and absence of chemically disturbing components are factors in support of the use of Citral in flavors, rather than in perfumes. Used in imitation Apple, Cherry, Ginger, Grape, Lemon, Lime, Orange, Grapefruit, Spice, Strawberry and even in Vanilla.

Concentration is normally about 40 ppm in the finished product, but can be up to 150-170 ppm in Chewing gum.

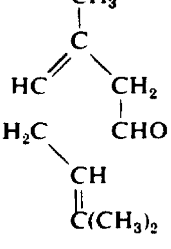
G.R.A.S. F.E.M.A. No.2303.

Prod.: many methods – the reader is referred to: 156-102ff.

See also literature: 26-464; 86-32; 100-265; 106-106; 156-99; 140-160; B-I-753;

## 650: iso-CITRAL

*3*,*7*-Dimethyl-*3*,*6*-octadienal.



$C_{10}H_{16}O = 152.24$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.87. B.P. approximately 214° C.

Floral-citrusy, delicate odor, very different from that of Citral. Sweeter, fresher than Citral, and more floral (Lily-like).

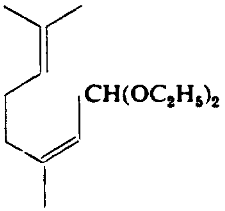
Suffering from the same instability drawbacks as Citral, this aldehyde has never achieved real popularity among perfumers. The production of *iso*-Citral involves the production of an intermediate derivative of Citral, and accordingly the cost of *iso*-Citral is always much higher than that of Citral, even though the odors can not be compared to one another.

Prod. from Citral enol acetate by reaction with Aluminum *iso*-propylate.

5-95; 86-73; 156-106;

## 651: CITRAL DIETHYLACETAL

*3*,*7*-Dimethyl-*2*,*6*-octadienal diethylacetal.
(Commercial products consist of approximately 70% Geranial diethylacetal and 30% Neral diethylacetal).
Main component:



$C_{14}H_{26}O_2 = 226.36$

Colorless, slightly oily liquid. B.P. a trifle higher than that of Citral.

Very slightly soluble in water, soluble in alcohol, fairly soluble in Propylene glycol, miscible with most perfume and flavor oils.

Mild and fresh, green-citrusy, almost vegetable-juicy odor with a pleasant, natural oily-fruity undertone. The odor is very heavily influenced by the presence of small amounts of Citral. Perhaps partly because acetals were not produced in a very pure state when they first appeared on the market, it has been more or less conventional that the odor of Citral diethylacetal has been described with phrases including those used for Citral.

NOTE: The human olfactory system is notoriously poor when it comes to estimating power or percentage of a powerful odor-component in a mixture or in a diluent.

5% Citral in Citral diethylacetal changes completely the odor picture and gives impression – to the unexperienced evaluator – of a much "stronger" chemical.

The acetal is used in perfume compositions, partly as a topnote ingredient in delicate floral fragrance types, and in the more modern green-fruity fragrances as a modofier to the conventional complex of alifatic aldehyde + Styrallyl esters + Galbanum, etc. Since it is stable in soap, it can be used in such fragrances, but should not be considered anything near a substitute for Citral as an odor.

Used in flavor compositions, mainly in Citrus flavors along with natural oils and synthetic flavor chemicals. It will introduce quite natural green-oily, "peel" notes in Lemon and Lime, and it can be twisted into an Orange with the proper background materials.

Concentration in the finished product is usually about 100 ppm in condiments, (lower in other products). It should be kept in mind that the acetal is NOT stable in acid media, and therefore does NOT perform with its acetal odor in an acidified soft drink or the like.

Prod. (several methods) e.g. from Ethyl orthoformate and Citral.

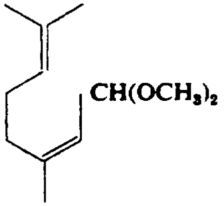
G.R.A.S. F.E.M.A. No.2304.

5-317; 86-32; 156-100; 156-106; 140-160;

## 652: CITRAL DIMETHYLACETAL

*3*,*7*-Dimethyl-*2*,*6*-octadienal dimethylacetal.
Consists of approximately 70% Geranial dimethylacetal and 30% Neral dimethylacetal.

(Main component)



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Sp.Gr. 0.89. B.P. slightly lower than that of Citral.

Almost insoluble in water, soluble in alcohol and oils.

Very mild, oily-green, vegetable-fresh and slightly citrusy odor.

Sweet and slightly citrusy taste with an "unripe-fruit"-freshness.

Used in perfume compositions partly as a mild-green topnote in soap fragrances, also as a topnote modifier in delicate floral fragrances, green-citrusy types, fresh notes, etc.

Used in flavor compositions mainly in Citrus types and generally in fruit flavors to introduce a natural freshness similar to that of unripe fruit or green Lemon peel, Apple peel, etc.

Concentration is usually about 55-65 ppm in candy or in baked goods.

NOTE: See NOTE under Citral diethylacetal (previous monograph).

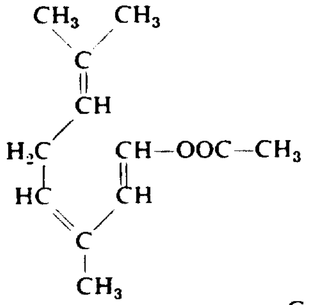
G.R.A.S. F.E.M.A. No.2305.

Prod. from Citral and Methanol with dry HCl-gas.

86-32; 106-109;

## 653: CITRAL ENOL ACETATE

Exists in *cis*- and *trans*-forms.
The commercial material is actually:
*iso*-Citral enol acetate:



$C_{12}H_{18}O_2 = 194.28$

Colorless, slightly oily liquid. Sp.Gr. 0.94.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, fruity-rosy odor, somewhat resembling that of Neryl acetate, but lighter and fresher of character.

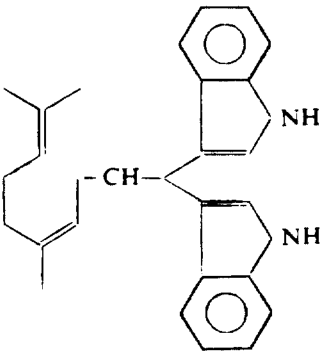
Has been suggested for use in perfume compositions as a modifier to the conventional "rose-alcohol"-esters. However, the poorer stability, the higher cost of the enol acetate, and the fact that there is already a very good selection of "rose-esters" on the perfumer's shelf, have more or less prevented the enol acetate from becoming a standard shelf item.

Prod. from Citral with Acetic anhydride and Sodium acetate (anhydr.).

86-32; 156-106;

## 654: CITRAL-INDOLE

A type of condensation product.
Structure formula (presumably):



Viscous, pale straw-colored liquid, insoluble in water, soluble in alcohol, miscible with perfume oils.

The material changes color upon standing, usually to the darker orange-reddish color shades.

Stability and odor type depends strongly upon the method of processing and the ratio of Citral/Indole used in the reaction.

Generally speaking, the condensation products of Citral with primary amine type chemicals (e.g. Anthranilates) and with secondary type chemicals (e.g. above product), are not very interesting, usually very dark colored and unstable.

It is most conceivable that the above product was developed in search of products with effects resembling that of Citronellal-Indole (see that monograph).

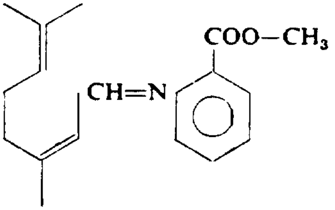
The author believes that the above product has no potential interest to perfumery.

Prod. by condensation of Citral with two mols. Indole.

(Private laboratory experiments).

## 655: CITRAL-METHYLANTHRANILATE

A "Schiff's base"-type of condensation product:



$C_{18}H_{23}NO_2 = 285.39$

Viscous, dark orange colored liquid, insoluble in water, soluble in alcohol, miscible with perfume oils.

The odor, which may vary from sweet Orange-blossom to fresh Orange peel-like, or Grapefruit-peel-like, is strongly dependent upon the method of preparation and the ratio of Aldehyde/Anthranilate used.

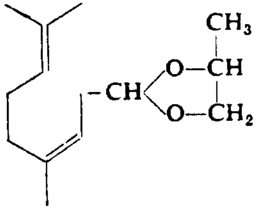
Being comparatively pale amber to orange colored when freshly prepared, this phoduct turns darker quickly, and causes considerable color difficulties in the composition in which it may be incorporated.

Most conceivably, this product can remain on the research shelf, or rather in the files. It does not contribute any highly interesting or indispensable notes to fragrance compositions.

Prod. by condensation of Citral with Methylanthranilate (equal mols.).

## 656: CITRAL PROPYLENEGLYCOL ACETAL

(A cyclic acetal).



$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid. Slightly soluble in water, soluble in alcohol and oils. The material shows slight decomposition when dissolved in water. It is also soluble in Propylene glycol.

Very pleasant, sweet-citrusy lemon-orange-like odor, mild, oily and somewhat green.

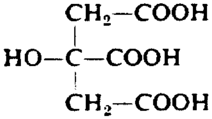
Pleasant, but rather weak lemony taste in aqueous media (the decomposition changes the flavor to lemon).

This acetal has been suggested for use in flavor compositions, but its instability presents a drawback, particularly since the purpose of using the acetal was to introduce a *different* and modifying flavor note - not the Citral note.

Prod. by condensation of Citral with Propylene glycol, using a catalyst.

## 657: CITRIC ACID

*2*-Hydroxy-*1,2,3*-propane tricarboxylic acid.
*beta*-Hydroxy tricarballylic acid.



$$\begin{array}{l} \quad\;\; CH_2—COOH \\ \quad\;\;\; | \\ HO—C—COOH \\ \quad\;\;\; | \\ \quad\;\; CH_2—COOH \end{array}$$

$C_6H_8O_7 = 192.13$
(anhydrous)

White crystalline powder. M.P. 153° C.

The product containing 1 Mol. water melts below 100° C.

Soluble 66% in water, 33% in alcohol, 3% in ether. Soluble about 20% in Propylene glycol.

Virtually odorless. The aqueous solution has a clean acid taste, pleasant in the concentration of 0.02 to 0.08%. When used in sugar-sweetened aqueous media, the concentration may be somewhat higher. Cane sugar will furthermore chemically neutralize a measurable amount of Citric acid, thereby reducing the acidity. Very widely used as an acidifier in Citrus and fruit flavors, not included in the flavor oil, but as an additive along with sweeteners and other water-soluble taste corrigentia.

The concentration in Candy may be about 4400 ppm, in chewing gum about 3700 ppm, and in various food products about 4200 ppm.

The annual world consumption of Citric acid in food products and candy amounts to tens of thousands of metric tons, or, in other words, enough to acidify several pounds of consumer product per person per year in the entire world.

G.R.A.S. F.E.M.A. No.2306.

Prod.

1) by isolation from Citrus fruit juices or Pineapple waste.
2) (mostly) by selective, controlled fermentation of crude sugar liquids with Aspergillus or other mycelia.

26-464; 77-190; 77-242; 100-266; 107-259; 157-319; B-III-464;

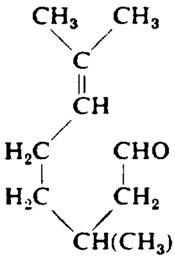
## 658: CITRONELLAL

*3*,7-Dimethyl-*6*-octen-*1*-al.

"Rhodinal" (incorrect name).

This chemical exists in *dextro-*, *laevo-* and *dl-(racemic)*-forms.

The *laevo*-form is the one referred to when the name "Rhodinal" is used. It is naturally occurring in the essential oils from leaves or peel of certain varieties of Grapefruit "pamplemousse").



$C_{10}H_{18}O = 154.25$

Colorless mobile liquid. Sp.Gr. 0.85.

B.P. 206° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, fresh, green-citrusy, slightly woody odor, lacking in sweetness and fruitiness as compared to Citral, and more suggestive of Citronella oil, inevitably if the observer is familiar with that oil.

This aldehyde is rather unstable under exposure to air, daylight and alkali, and is therefore not much used as such in perfumes or flavors. Citronella oil is less expensive and more stable. It gives a more attractive picture of the Citronellal odor in its natural modification and composition.

Citronellal is occasionally used – in traces – in flavor compositions of the Citrus, Cherry, Fruit (tutti-frutti), Ginger Ale, Spice and other types.

G.R.A.S. F.E.M.A. No.2307.

Prod. (many methods) e.g.:

1) By isolation from Eucalyptus Citriodora oil or from Java/Formosa/Guatemala type of Citronella oil.
2) Synthetically from Pinene.
3) By dehydrogenation of Geraniol.

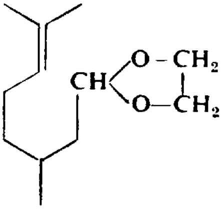
5-98; 86-32; 104-228; 104-189; 106-110; 89-52; 156-112; 26-464; B-I-745;

## 659: CITRONELLAL CYCLOMONOGLYCOLACETAL

Citronellal ethyleneglycolacetal.

A cyclic acetal.

The title name is commonly used in perfumery literature.



$C_{12}H_{22}O_2 = 198.31$

Colorless viscous liquid. Very slightly soluble in water, soluble in alcohol and oils.

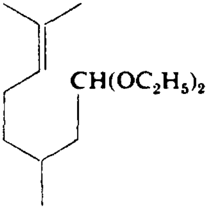
Mild, green-herbaceous and sweet odor of considerable tenacity. Commercial products vary in odor type and strength, probably because of differences in composition and purity.

This acetal has been suggested for use in perfume compositions as a novel note in fresh-floral and citrusy-herbaceous fragrance types.

However, its cost does not allow for very liberal use of this material in the common perfumes for household products, etc., where the odor would most likely find acceptance. Other materials can yield more odor at less cost, and the title material will probably never enter the perfumer's routine library of materials.

Prod.: by condensation of Citronellal and Ethyleneglycol.

## 660: CITRONELLAL DIETHYLACETAL



$C_{14}H_{28}O_2 = 228.38$

Colorless liquid. Sp.Gr. 0.86. B.P. 232° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and most perfume oils.

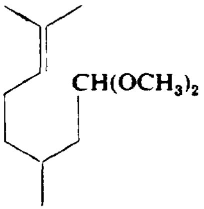
Very faint odor when absolutely pure (free from Aldehyde). More lemony-green than the aldehyde proper.

The parent aldehyde has very little use as such in perfumery, and the acetal even less. Beyond some academic interest, there is probably very little, if any at all, demand for this acetal in perfumery.

Prod. from Citronellal plus Ethyl-*ortho*-formate plus a catalyst in Ethyl alcohol.

5-317; 86-32;

## 661: CITRONELLAL DIMETHYLACETAL



$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Sp.Gr. 0.93. B.P. 221° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and perfume oils.

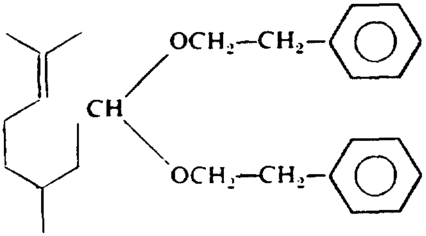
Very faint, grassy-green, slightly lemony-oily odor. The pure acetal has only very little odor at all.

Beyond some academic interest, there is probably no demand for this acetal for use in perfumes or flavors. It does not offer any interesting notes unobtainable by other means, and it does not contribute power or character to a fragrance.

Prod. from Citronellal plus Methanol plus Formimino methylether.

5-316; 86-33;

## 662: CITRONELLAL DI-PHENYLETHYL ACETAL



$C_{26}H_{38}O_2 = 380.57$

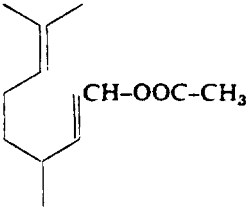
Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Very faint, soft-floral-fresh odor of good tenacity. The odor varies considerably in samples from different sources, most conceivably because of contamination with one or the other component of the acetal. It has been claimed that the pure acetal is virtually odorless to the human nose.

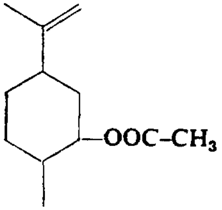
Of little, if any interest at all to perfumery.

## 663: CITRONELLAL ENOL ACETATE

The commercial products always contain some *iso*-Pulegyl acetate.



Citronellal enol acetate



*iso*-Pulegyl acetate

$C_{12}H_{20}O_2 = 196.19$

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Fresh-green-citrusy, almost herbaceous odor, usually contaminated with a Dill-weed like odor from *iso*-Pulegyl acetate.

This enol acetate is rather unstable on storage, and has never achieved much popularity among perfumers, mainly because of its variable odor and progressive deterioration.

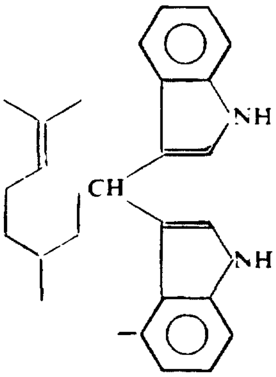
It forms an interesting member of intermediates in the processes of making *iso*-Pulegol, *iso*-Pulegone, Menthol, etc.

Prod. by Acetylation of Citronellal with Acetic anhydride and Sodium acetate (anhydrous) *at low temperature.*

5-101; 86-33; 156-115;

## 664: CITRONELLAL-INDOLE

A condensation product, presumably of the structure:



$C_{26}H_{28}N_2 = 368.53$

Very viscous, straw-colored liquid. Insoluble in water, soluble in alcohol and most perfume oils. Almost insoluble in Propylene glycol.

Fresh-floral and very tenacious odor, recalling the delicate as well as the deep-exotic notes from natural flower material, mostly in Jasmin-Tuberose direction.

The odor of the material itself is strongly dependent upon the method of preparation and the ratio of Aldehyde to Indole used, but the effect in actual application does not seem to vary so considerably, as long as the bulk of the material is really one component. However, it is important that an eventual surplus of Indole be controlled and kept at a reasonably low level.

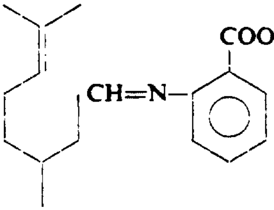
This product finds use in the creation of floral bases, where a certain amount of Indole is desirable, yet the effect of so much free Indole is not wanted. In other words, the product may serve as a battery of Indole for slow and continuous release of indolic notes at a more desirable level.

Prod. from Indole and Citronellal by condensation in the ratio of 2 mols. Indole to 1 mol. Citronellal. The condensation may be carried out in an inert odorless solvent.

(Partly based upon private experiments).

## 665: CITRONELLAL-METHYLANTHRANILATE

A "Schiff's base" type of condensation product.



$C_{18}H_{25}NO_2 = 287.41$

Very viscous pale amber, dark amber or brownish-amber colored liquid (pale when freshly prepared). Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Very tenacious, sweet-floral, Orange-peel and Orange-blossom complex odor. Fresher than the classic "H.M.A." it does not have the Honeysuckle sweetness of that material. while it presents more Orange-rind notes.

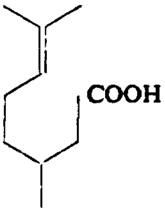
Not quite as versatile as its ancestor, Hydroxycitronellal-Methylanthranilate, it has never achieved much popularity. It also seems to produce more of a color problem, and its odor does change upon storage or ageing.

Produced by condensation of equal mols. of Citronellal and Methyl anthranilate.

(Partly based upon private experiments).

## 666: CITRONELLIC ACID

Rhodinolic acid.
*3,7*-Dimethylocten-*6*-oic acid-*1*.



$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. Sp.Gr. 0.93. B.P. 252° C.

Almost insoluble in water, soluble in alcohol and oils.

Faint, fresh-green, somewhat grassy odor, not very pleasant, rather weedy-oily note.

Has been suggested for use in the "reconstruction" of certain essential oils, and since the acid is commercially available, although not very regularly, there is some reason to believe that it may be of interest for these specific purposes.

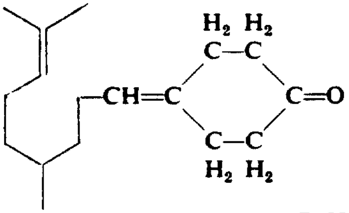
The future outlook for essential oils as basic perfume raw materials is not the best. and it will remain a perfumer's job to keep on shelf a series of good substitute oils in case of sudden shortage of the natural material.

Prod. by oxidation of Citrone*llol* with Chromic acid, or by oxidation of Citrone*llal* with Silver oxide.

90-130;

## 667: CITRONELLIDENE CYCLOHEXANONE

*3*-Citronellidene-cyclohexanone.



$C_{16}H_{26}O$ = 234.38

Colorless liquid.

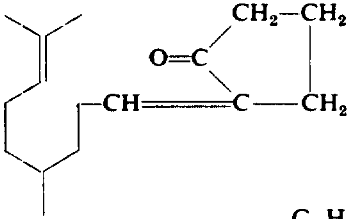
Insoluble in water, soluble in alcohol, miscible with perfume oils.

Powerful, spicy-weedy, somewhat camphoraceous odor. However, the overall picture is not that of an attractive odor, it is rather nondescript and does not call any distinct, natural odor to one's mind.

The material has probably only academic interest today.

Prod. from Citronellal and Cyclohexanone by condensation.

## 668: alpha-CITRONELLIDENE CYCLOPENTANONE



$C_{15}H_{24}O$ = 220.36

Colorless liquid. Insoluble in water, soluble in alcohol, miscible with perfume oils.

Powerful weedy-camphoraceous-minty odor with a herbaceous undertone, including some sweetness, but not enough to call the material overall pleasant smelling.

Has been suggested for use in perfume compositions, but could possibly only find some use in artificial essential oils, e.g. Geranium.

However, the author believes that this material will have only academic interest in the future.

Prod. by condensation of Citronellal with Cyclopentanone.

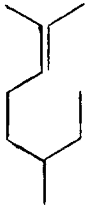
## 669: CITRONELLOL

*dl*-Citronellol (commercial C. is usually racemic).

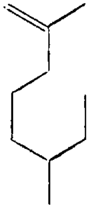
*3,7*-Dimethyl-*6*-octen-*1*-ol.

Cephrol (ABRAC).

Commercial Citronellol usually contains measurable amounts of Geraniol and variable amounts of Dimethyl octanol (up to 15%).



*alpha*-Citronellol
(in natural prod.)



*beta*-Citronellol
(synthetic Citr.)
Occurs only rarely
in natural prods.

$C_{10}H_{20}O$ = 156.27

Colorless liquid. Very slightly soluble in water, soluble in alcohol, miscible with perfume and flavor oils. Soluble in Propylene glycol, but not in Glycerin. Sp.Gr. 0.86. B.P. 225° C.

Fresh rosy odor, variable according to purity, content of Dimethyloctanol, Geraniol, etc. Overall sweet, fresher, lighter rosy-floral than Geraniol.

Floral-rosy, but rather bitter taste in aqueous media.

Very extensively used in perfume compositions, not only for rosy fragrance types, but in general as a fresh-floral, chief ingredient of a multitude of soap fragrances, household product fragrances, low cost perfumes, etc. It may be a major ingredient in low-cost Muguet types, and together with Geraniol, Phenylethyl alcohol, etc. form the basis of most Rose fragrances.

Used in flavor compositions for imitation Berry, Citrus, Fruit, Floral, Rose-, Raspberry, Strawberry and occasionally Peach.

Concentration may be about 16-20 ppm in baked goods, and as high as 50 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2309.
FCC-1964-807.

Prod. (several methods) e.g.:

1) from Citronella oil by hydrogenation of the Geraniol component.
2) from Pinene (in the synthesis of Hydroxycitronellal).
3) from Citronellal by reduction (this yields a very pure Citronellol).

4-33; 26-464; 77-172; 87-492; 106-111; 156-120; B-I-451; 140-126;

## 670: laevo-CITRONELLOL

"Rhodinol" (misleading name).
"Levocitrol" (Firmenich).

The perfume material generally marketed under the name "Rhodinol" (see that monograph) is not a well-defined or single chemical. It is a mixture almost exclusively consisting of alcohols from Geranium oil after saponification. The saponified oil is submitted to fractionated vacuumdistillation and fractions selected by olfactory means are composited into the product known as "Rhodinol ex Geranium".

That product consists mainly of *dextro*-Citronellol, some *laevo*-Citronellol, plus smaller amounts of Linalool, *4*-Terpinenol, Phenylethyl alcohol, *cis-3*-Hexenol, etc.

"Rhodinol" is, however, also used as a trade name for a purified synthetic or isolated *laevo*-Citronellol.

An odor description of *laevo*-Citronellol would therefore refer to the latter category only:

Colorless oily liquid of very fresh, light and quite diffusive, rosy-leafy, slightly waxy, petallike odor. It is sweeter than ordinary Citronellol, and has absolutely no "minty" notes, yet a certain "coolness" in its fresh odor.

The taste is deficient in sweetness and needs very strong support of sweetening flavor ingredients to become overall attractive, nonperfumey.

*laevo*-Citronellol is used in perfume compositions where it is of paramount importance that the natural rosy notes are conspicuous, lifting and clean-fresh. The *laevo*-Citronellol stands out primarily by showing a clean "peak" of fresh-rosy topnote, where the ordinary racemic Citronellol will show dullness and lack of "topnote-effect".

Prod.

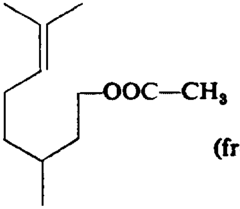
1) by isolation from Bulgarian Rose oil (this will yield *laevo-beta*-Citronellol).
2) by reduction of *laevo*-Citronellal from Combava-petitgrain oil (this yields mostly *laevo-alpha*-Citronellol).
3) from Methyl heptenol via the Bromide, reacted with Magnesium, then treated with Ethylene oxide. Hydrolysis of the reaction product yields Rhodinol.

And a number of other methods are patented.

5-26; 87-492; 106-114; 156-120;

## 671: CITRONELLYL ACETATE

"Cephreine" (A.B.R.A.C.).
*3*,*7*-Dimethyl-*6*-octen-*1*-yl acetate.



(from natural Citronellol)

$C_{12}H_{22}O_2 = 198.31$

Colorless, slightly oily liquid. Sp.Gr. 0.89. B.P. 229° C.

Almost insoluble in water, Propylene glycol and Glycerin, soluble in alcohol and oils.

Fresh-rosy-fruity odor, somewhat reminiscent of Geranium.

Fruity-rosy taste, but not sweet enough to be truly pleasant.

Extensively used in perfume compositions for Rose, Lavender, Muguet, Lily, Peony, Geranium, Bergamot- and Citrus-Colognes, etc. Stable in soap, does not discolor.

Frequently used in flavor compositions for imitation Apple, Apricot, Banana, Cucumber, Gooseberry, Grape, Lemon, Pear, Quince, Raisin, Rose, etc.

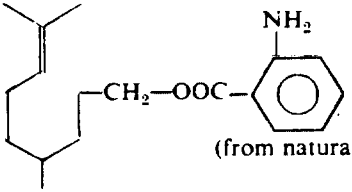
Concentration will in most cases be traces only (a few ppm in the finished product), but may be up to 600-700 ppm in chewing gum.

Prod. from Citronellol and Acetic anhydride (Acetylation).

G.R.A.S. F.E.M.A. No.2311.
FCC-1964-809.

4-33; 77-183; 86-33; 90-245; 106-115; 156-126; 140-136;

## 672: CITRONELLYL ANTHRANILATE



(from natural Citronellol)

$C_{17}H_{25}NO_2 = 275.40$

Almost colorless or slightly straw-colored, viscous liquid. B.P. 365° C. Sp.Gr. 1.06.

Insoluble in water, soluble in alcohol, miscible with perfume oils. Insoluble in Propylene glycol and Glycerin.

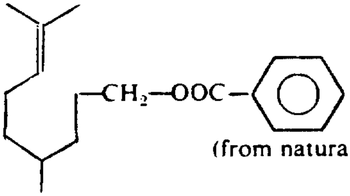
Rich, sweet, floral-rosy, fruity odor of considerable tenacity. The odor varies according to the origin of the sample (method of preparation), age, etc. The author believes however, that esters prepared by the more modern method (below) show less "Orangeblossom" character, and more of a generally floral, intensely sweet, slightly fruity character.

This ester is not a very common commercial article, and may never become a standard item on the perfumer's shelf. Skilful use of a combination of other esters and perfume materials can produce almost identical odor effects, and it is therefore doubtful whether this ester can survive.

Prod. from Isatoic anhydride and Citronellol.

34-1011; 34-1022;

## 673: CITRONELLYL BENZOATE



(from natural Citronellol)

$C_{17}H_{24}O_2 = 260.38$

B.P. 340° C. Sp.Gr. 0.98.

Colorless viscous liquid, or pale straw-colored liquid. Insoluble in water, soluble in alcohol, miscible with oils. Almost insoluble in Propylene glycol.

Very mild rosy, somewhat dry-woody odor of considerable tenacity, but of low odor value, overall not too interesting.

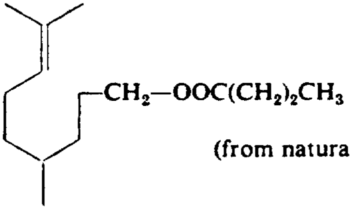
Occasionally used as a fixative in Hyacinth, Rose or Muguet fragrances.

Prod. by direct esterification of Citronellol with Benzoic acid under azeotropic conditions and using a catalyst.

4-33; 86-33;

## 674: CITRONELLYL BUTYRATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl-*n*-butyrate.



(from natural Citronellol)

$C_{14}H_{26}O_2 = 226.36$

Colorless liquid. Sp.Gr. 0.88. B.P. 245° C.

Almost insoluble in water, soluble in alcohol and oils.

Intensely fruity, sweet and somewhat rosy, leafy (rose-petal-like) odor. Overall warm, deep and very pleasant. However, traces of free acid in deteriorated or poor-grade products completely ruin the odor picture. The ester is surprisingly stable once it is produced acid-free and moisture-free.

Sweet, deep-rosy-fruity taste, reminiscent of Apple and Rose.

Used in perfume compositions for Muguet, Lavender, Rose (leaf-notes, Eglantine-notes, fruity Rose-notes, etc.), and as a modifier for lower esters of Citronellol.

Used in flavor compositions for imitation Apple, Banana, Cola, Honey, Pineapple, Plum, Prune, and in Rose and various floral types of flavor bases.

Concentration is usually limited to a few ppm in the finished product (traces).

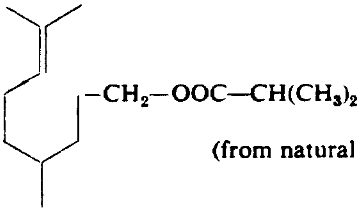
Prod. by direct esterification of Citronellol with Butyric acid under azeotropic conditions, or with Butyric anhydride.

G.R.A.S. F.E.M.A. No.2312.

4-33; 77-186; 86-33; 90-270; 106-116; 156-124; 5-233; 140-140;

## 675: CITRONELLYL-iso-BUTYRATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl-*iso*-butyrate.



(from natural Citronellol)

$C_{14}H_{26}O_2 = 226.36$

Colorless liquid. Almost insoluble in water and Propylene glycol, soluble in alcohol and oils. Sp.Gr. 0.88. B.P. 249° C.

Fresh, almost citrusy-rosy, intensely fruity and sweet odor, lighter than that of the *n*-Butyrate, not as warm or deep.

Fruity-rosy, somewhat Bergamot-like taste of modest sweetness.

Used in perfume compositions for Geranium, Rose, Muguet, Freesia, Peony, Acacia, Lilac, Hyacinth, Bergamot, etc. and as a modifier for lower esters of Citronellol in floral and fruity-floral, sweet fragrance types.

Used in flavor compositions for imitation Grape, Quince, Raspberry, Strawberry, Rose, and in a variety of "floral" flavor types.

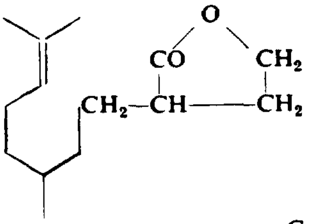
Concentration is usually only traces (a few ppm) in the finished product.

Prod. by direct esterification of Citronellol with *iso*-Butyric acid under azeotropic conditions, or with *iso*-Butyric anhydride.

G.R.A.S. F.E.M.A. No.2313.

4-34; 5-233; 77-186; 86-34; 106-118;

## 676: alpha-n-**CITRONELLYL**-gamma-**BUTYROLACTONE**



$C_{14}H_{24}O_2 = 224.35$

Almost colorless, viscous or oily liquid.

Insoluble in water, soluble in alcohol, miscible with perfume oils.

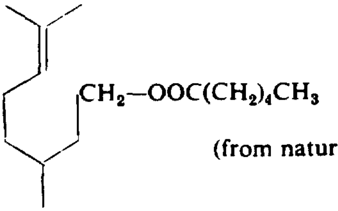
Faint, but rather heavy and very tenacious, musky-fruity odor of Pear-Peach type with somewhat dry undertones (musky).

Has been suggested for use in perfume compositions, but the author feels that this material has little more than academic interest to the perfumer of to-day.

30-254; 31-170; 159-418;

## 677: CITRONELLYL CAPROATE

Citronellyl hexylate.
Citronellyl hexoate.



(from natural Citronellol)

$C_{16}H_{30}O_2 = 254.42$

Colorless liquid, insoluble in water, soluble in alcohol and perfume oils. Sp.Gr. 0.88.
B.P. 240° C.

Delicately floral, pronounced fruity (Apple-Pear-Pineapple notes) and somewhat rosy odor of fair tenacity.

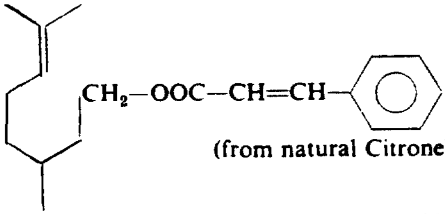
The taste is not too attractive, since the bitterness of the Citronellol component seems to come through.

Occasionally used in perfume compositions as a modifier for lower esters of Citronellol, and in certain mild-floral fragrance types, Peony, Freesia, Sweet Pea, etc. It is also interesting in lipstick perfumes where the conventional Ionone-fruitiness certainly needs some renewal in notes.

Prod. by direct esterification of Citronellol with Caproic acid under azeotropic conditions.

4-34; 34-1230; 86-33; 90-278;

## 678: CITRONELLYL CINNAMATE



(from natural Citronellol)

$C_{19}H_{26}O_2 = 286.42$

Colorless oily liquid. B.P. 380° C.
Sp.Gr. 0.99.

Insoluble in water, soluble in alcohol and perfume oils.

Very faint, sweet-floral and somewhat oily odor of great tenacity.

Actually of very little interest, this ester is occasionally used and has been suggested as a blender for Hydroxycitronellal, Bucinal, Cyclamal, etc. in delicate floral fragrances. It will also act as a fixative, but its odor contribution is almost nil.

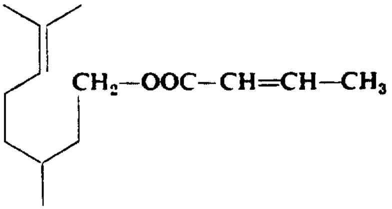
It has a tendency to polymerize, whereby it turns absolutely odorless (and cloudy-viscous), depending upon the method of preparation and added inhibitors.

Prod. by direct esterification of Citronellol with Cinnamic acid and a catalyst under azeotropic conditions, or: from Cinnamyl chloride plus Citronellol and a catalyst.

4-33; 34-484; 86-33;

## 679: CITRONELLYL CROTONATE

Citronellyl-*2*-butenoate.
Citronellyl-*alpha*-crotonate.



$C_{14}H_{24}O_2 = 224.35$

Colorless or pale straw-colored oily liquid. Insoluble in water, soluble in alcohol and oils.

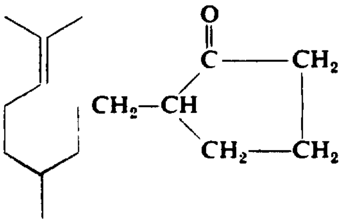
Fresh-herbaceous, slightly green and warm-rosy odor of moderate tenacity. A winey note seems to be normal in this ester.

Rarely offered commercially, this ester has been suggested for use in floral and herbaceous fragrances, including better soap perfumes. It has considerable power and good effect in soap, but there are many related chemicals, some less expensive, others more freely available, with similar effects.

It serves – like Geranyl crotonate – as an extender for Geranium and it can support Lavender and Clary Sage notes as well.

Prod.: by direct esterification of Citronellol with *2*-Butenoic acid under azeotropic conditions.

## 680: alpha-CITRONELLYL CYCLOPENTANONE



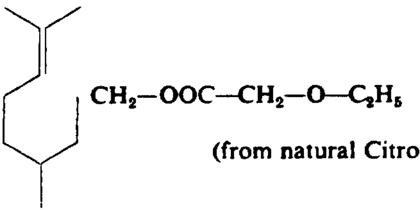
$C_{15}H_{26}O = 222.37$

The above material has been reported as being an interesting perfume material with a floral, sweet-rosy and deep, lasting odor.

The author is not aware of any extensive or common use of this material in perfumery, under its proper chemical name, or under cover of a trade name.

Prod. by hydrogenation of Citronellidene cyclopentanone (see that monograph).

## 681: CITRONELLYL ETHOXYACETATE



(from natural Citronellol)

$C_{14}H_{26}O_3 = 242.36$

This material has been reported as being a potential perfume chemical.

Its odor has been described as sweet rosy, more honeylike and longer lasting than that of the Acetate.

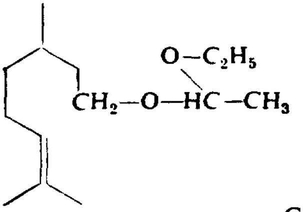
The author believes that this chemical is rarely, if ever, used in perfumery, and that its odor is not interesting enough to justify its existence as another shelf-item for the creative perfumer.

Prod. from Ethoxyacetic acid plus Citronellol with a catalyst under azeotropic conditions.

31-159;

## 682: CITRONELLYL ETHYL ACETAL

The title name is a commercial name.
Ethyl citronellyl acetal (modern chemical name).
Acetaldehyde ethyl-citronellyl acetal (correct chemical name).
A "mixed" acetal.



$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet, delicately green-leafy-oily odor with a fruity note. Much sweeter than the Citronellyl methyl acetal (see monograph).

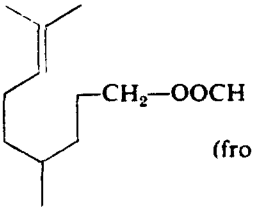
Moderate to good tenacity.

The title acetal has been suggested for use in perfume compositions for its refreshing and discrete notes, blending equally well with floral and herbaceous or citrusy fragrance types. It is particularly suitable for topnote compositions in connection with Bergamot or Neroli, and it has a very pleasant effect upon Cyclamen aldehyde.

The material is rarely offered commercially, but often prepared by the interested party for use in bases or specialties.

Prod. (several methods) e. g. from Acetaldehyde diethylacetal (= "Acetal") with Citronellol.

## 683: CITRONELLYL FORMATE



(from natural Citronellol)

$C_{11}H_{20}O_2 = 184.28$

This ester is, in the author's opinion, by far the most interesting of all the Citronellyl-esters. Sp.Gr. 0.89-0.90. B.P.235° C.

Very slightly soluble in water, poorly soluble in Propylene glycol, insoluble in Glycerin, soluble in alcohol, miscible with perfume and flavor oils.

Colorless mobile liquid, powerful leafy-green, fruity-rosy, fresh and light odor reminiscent of Geranium leaves, somewhat dry and honeylike undertone. There is an overall fresh-vegetable character in this odor picture.

Extensively used in perfumery, particularly since it is amazingly stable even in soap, as a Geranium note, as a lifting topnote, in support of Bergamot or other Citrus-notes, Lavender notes, in Oriental fragrances (it blends surprisingly well with Patchouli and Olibanum), and to freshen the Phenylacetic notes in honey-odors. Also with Cyclamal in "Cucumber"-notes.

Used in flavor compositions for imitation Apple, Apricot, Cucumber, Honey, Orange, Peach, Plum, etc.

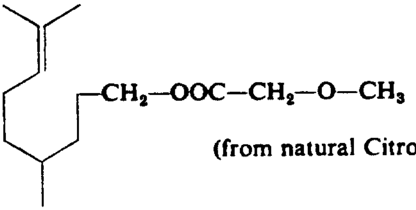
Concentration is normally about 40 ppm, but can be up to 100 ppm in chewing gum.

G.R.A.S. F.E.M.A. FCC-1964-811.

Prod. from Citronellol and excess Formic acid (by hot or cold process).

4-33; 5-247; 77-179; 86-33; 90-239; 106-117; 140-132;

## 684: CITRONELLYL METHOXYACETATE



(from natural Citronellol)

$C_{13}H_{24}O_3 = 228.34$

This ester has been reported as a chemical with potential interest to the perfumer.

Its odor has been described as sweet-rosy, somewhat green, fresh and honeylike, longer lasting than that of the Acetate.

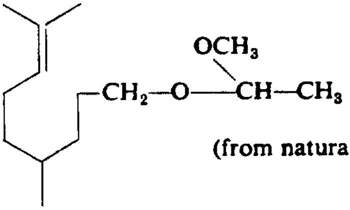
The author feels that this ester – like the Ethoxyacetate – has little to offer to the creative perfumer, and that it will not become a standard item on his shelf.

31-159;

## 685: CITRONELLYL METHYL ACETAL

*(commercial name)*

A "mixed" acetal.
Methyl citronellyl acetal (modern chemical name).
Acetaldehyde citronellyl methyl acetal.



(from natural Citronellol)

$C_{13}H_{26}O_2 = 214.35$

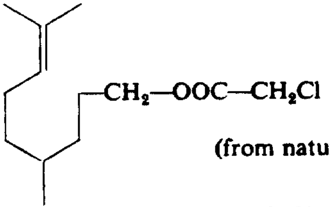
Colorless mobile liquid. Almost insoluble in water, soluble in alcohol and oils.

Green-leafy, Geranium-Rose type odor, diffusive, fresh and natural. Somewhat reminiscent of Citronellyl vinyl ether (see that monograph).

Used in perfumery in support of Geranium notes, particularly in better soap perfumes, etc. It can also be considered as a variation of the Citronellyl formate theme, and used as a modifier for the lower esters of Citronellol.

Prod. from Citronellol plus Methanol plus Acetaldehyde. More commonly from Citronellol plus Acetaldehyde dimethylacetal.

## 686: CITRONELLYL MONOCHLOROACETATE



(from natural Citronellol)

$C_{12}H_{21}ClO_2 = 232.76$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very faint, sweet-rosy, deep and tenacious odor.

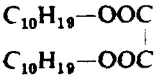
Has been suggested for use in perfume formulations as a fixative-modifier in Muguet, Rose, Peony, etc.

The author feels that the creative perfumer can easily be without this chemical, and there is a general aversion against the use of chlorinated chemicals, even those where the chlorine is safely locked in.

Prod. by direct esterification of Citronellol with Monochloroacetic acid under azeotropic conditions.

4-34;

## 687: CITRONELLYL OXALATE



$$\begin{array}{l} C_{10}H_{19}\text{—OOC} \\ \quad\quad\quad\quad\;\; | \\ C_{10}H_{19}\text{—OOC} \end{array}$$

$C_{22}H_{38}O_4 = 366.55$

Colorless oily liquid. Sp.Gr. 0.95.

Very faint floral-rosy odor.

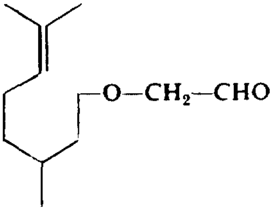
Has been suggested for use in perfumery as a fixative. The author feels that it has little, if anything at all, to offer of interest to the perfumer.

Prod. by direct esterification of Citronellol with Oxalic acid, using a catalyst (e.g. Toluene sulfonic acid).

4-34;

## 688: CITRONELLYL OXYACETALDEHYDE

"Muguet aldehyde" (I.F.&F.).
*6,10*-Dimethyl-*3*-oxa-*9*-undecenal.
Commercial products contain significant amounts of the Geranyl-isomer. The "Rhodinol"-oxyacetaldehyde is also known.



$C_{12}H_{22}O_2 = 198.31$

Colorless, viscous liquid. B.P. 239° C. Sp.Gr. 0.895.

The aldehyde is conventionally sold in reduced strength, either 50% or 70% aldehyde content. The diluent may be the corresponding acetal, or an odorless solvent, e.g. Diethylphthalate.

Insoluble in water, soluble in alcohol and perfume oils.

Powerful and moderately diffusive green-rosy, sweet Lily-Muguet-like odor. Its tenacity is comparatively good.

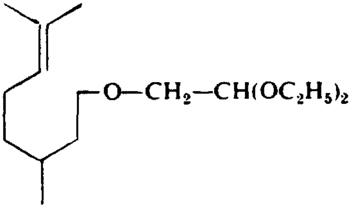
Used in perfume compositions as a floralizing aldehydic topnote ingredient, primarily in Muguet-Lily fragrances, but also in Rose, Peony (where the Geranyl-isomer is claimed to be superior), and various modifications of modern-aldehydic fragrance types.

Occasionally used in flavor compositions for floral or fruity types, and in Rose type flavors. The concentration is usually mere traces in the finished product.

Prod. from Citronellol, reacted with Sodium methylate or Sodium *iso*-propylate. The acetal is then prepared by reaction with Chlorodimethylacetal. The resulting acetal is finally hydrolyzed with diluted oxalic acid to yield the aldehyde.

86-34; 156-378;

## 689: CITRONELLYL OXYACETALDEHYDE DIETHYLACETAL



$C_{16}H_{32}O_3 = 272.43$

Colorless, slightly viscous liquid. B.P. 256° C. Sp.Gr. 0.89.

Very faint, delicate, Rose-Muguet type odor. Somewhat more oily, also more tenacious than the aldehyde, but much weaker.

The acetal is stable in mild alkali, and has therefore been suggested as a stabilizer for the aldehyde to extend the use of the much more powerful aldehyde.

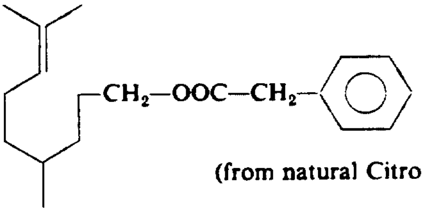
In itself the acetal does not contribute much odor and has apparently no other mission in perfumery than that of accompanying and protecting the aldehyde.

Prod. – see Citronellyl oxyacetaldehyde.

5-317; 86-34; 156-378;

## 690: CITRONELLYL PHENYLACETATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl phenylacetate.
(See also "Rhodinyl"-phenylacetate).



(from natural Citronellol)

$C_{18}H_{26}O_2 = 274.41$

Colorless, somewhat viscous liquid.
B.P. 342° C. Sp.Gr. 0.99.

Insoluble in water, soluble in alcohol and perfume oils.

Sweet-herbaceous-rosy, yet heavy and very tenacious odor, reminiscent of the petals of Roses, the waxy-honeylike, deep-sweet odor.

An excellent fixative-blender in many floral fragrances, particularly in Neroli-Orange-blossom, but also in non-florals, Oriental fragrance types, etc. It blends beautifully with Patchouli and Geranium, and it is extremely stable in soap and powders. However, the chemical purity and the odor quality of the material must be impeccable in the first place, or else the ester may break down just enough to produce unpleasant notes.

Used in flavor compositions for a variety of purposes: imitation Butter, Caramel, 'Fruit, Honey, Rose, etc. and in Tobacco flavoring.

Concentration in the finished product is usually mere traces (a few ppm).

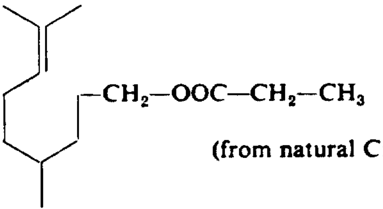
G.R.A.S. F.E.M.A. No.2315.

Prod. from Citronellol and Phenylacetyl chloride – or: by direct esterification of Citronellol with Phenylacetic acid using a catalyst under azeotropic conditions.

4-34; 34-246; 86-34;

## 691: CITRONELLYL PROPIONATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl propionate.



(from natural Citronellol)

$C_{13}H_{24}O_2 = 212.33$

Colorless liquid. B.P. 242° C. Sp.Gr. 0.88.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-fruity, sweet-rosy odor, richer, rounder than that of the acetate, also more berry-like, fruity.

Used quite frequently, but in modest concentrations, in many floral fragrance types, Rose, Muguet, Neroli, etc. and in Citrus types, particularly with Bergamot or Bergamot-like chemicals.

It has a pleasant effect upon Patchouli oil and is generally used as a modifier for the acetate, and for the esters of Linalool and Geraniol.

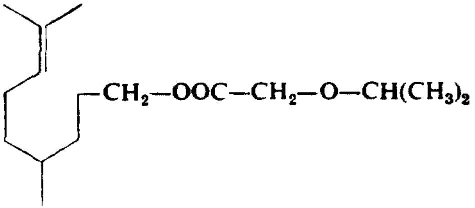
In flavor compositions, it finds its way into Lemon and various fruit flavors. The concentration in baked goods can be about 20 ppm.

G.R.A.S. F.E.M.A. No.2316.

Prod. by direct esterification of Citronellol with Propionic acid under azeotropic conditions, or with Propionic anhydride directly.

4-34; 33-622; 86-34; 106-119;

## 692: CITRONELLYL-iso-PROPOXYACETATE



$C_{15}H_{28}O_3 = 256.39$

Colorless liquid.

Reported as being a chemical of potential interest to the perfumer.

The odor has been described as fresh-fruity-rosy, more powerful than that of the esters of lower alifatic acids, somewhat less sweet, more rosy, less fruity, and more tenacious.

However, the entire odor picture does not include any distinct or unique notes unobtainable by other means, and the author feels that this ester can remain on the research shelf rather than enter the perfumer's laboratory.

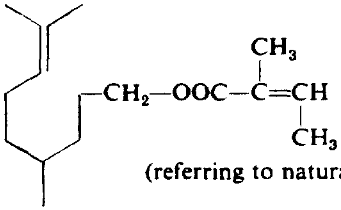
See also: Citronellyl ethoxyacetate and Citronellyl methoxyacetate.

31-159;

## 693: CITRONELLYL TIGLATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl-*trans-alpha*-methyl crotonate.

Citronellyl-*trans-alpha-beta*-dimethylacrylate.



(referring to natural Citronellol)

$C_{15}H_{26}O_2 = 238.37$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and perfume oils.

B.P. 267° C.

Somewhat dry, but very "natural" leafy-rosy, deep and slightly floral-balsamic odor. The word "balsamic" should be taken as an extension of "herbaceous" in the direction of deep sweetness, resembling the undertones in Clary Sage, etc.

There are some fruity notes in this ester, but they are not dominating the picture.

Probably forced out of research on Geranium components, this ester does not seem to be vitally important to the reconstruction of Geranium bases. However, it is in itself an interesting perfume chemical with possible application in herbaceous – sweet – tobacco-like or honeylike odor complexes.

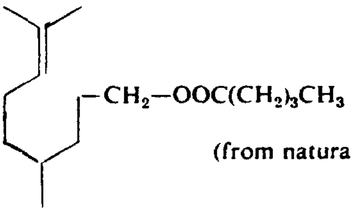
When used for Geranium and Rose bases, it may introduce notes resembling the undertones in absolute extracts of those botanicals.

Prod. from Citronellol with Tiglylchloride plus a catalyst in a low-boiling hydrocarbon solvent.

90-277;

## 694: CITRONELLYL VALERATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl-*n*-pentanoate.



(from natural Citronellol)

$C_{15}H_{28}O_2 = 240.39$

Colorless slightly oily liquid. B.P. 237° C. Sp.Gr. 0.88.

Insoluble in water, almost insoluble in Propylene glycol, soluble in alcohol, miscible with perfume oils and most flavor materials.

Warm-fruity, somewhat herbaceous, slightly rosy odor with undertones reminiscent of dried herbs or tobacco leaves, also slightly honey-like.

Deep-herbaceous, not very sweet, but pleasant honey-tobaccolike, somewhat fruity taste.

Used in perfume compositions as a modifier with lower esters of Citronellol. Also in support of Benzyl valerate, Linalyl-valerate, etc. in honeylike or tobaccolike notes. It seems to introduce more herbaceous-rosy notes than floral notes.

Occasionally used in flavor compositions – in traces only – for imitation Honey, Apple, Apricot, Pear, in tutti-frutti, etc.

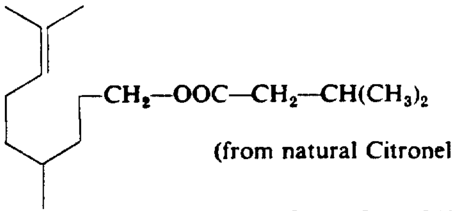
G.R.A.S. F.E.M.A. No.2317.

Prod. by direct esterification of Citronellol with *n*-Valeric acid under azeotropic conditions.

4-34; 86-34; 90-275; 5-238;

## 695: CITRONELLYL-iso-VALERATE

*3*,*7*-Dimethyl-*6*-octen-*1*-yl-*iso*-pentanoate.



(from natural Citronellol)

$C_{15}H_{28}O_2 = 240.39$

Colorless, slightly oily liquid. B.P. 253° C. Sp.Gr. 0.88. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol, miscible with most perfume and flavor oils.

Warm-rosy, herbaceous, chamomile-like, tobacco-like and very tenacious odor.

Useful in perfume compositions as a modifier for lower esters of Citronellol, and as a more herbaceous Rose-note in Oriental or Chypre type fragrances, Tabac-notes, etc. Also an interesting item in honey-like notes. It blends excellently with Civet products and emphasizes the pleasant notes in the Civet, subdueing the more unpleasant notes. Surprisingly stable in soap and even in Talcum powder.

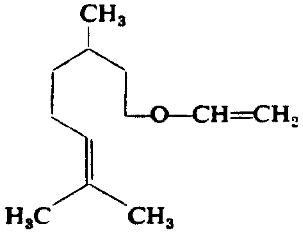
Occasionally used in flavor compositions, mainly for variations in Strawberry and Raspberry types. It is particularly useful in the "Wild Strawberry" type of flavor, along with Butyrates and Caproates.

(G.R.A.S.?) it is most conceivable that the "valerate" of commerce is actually the *iso*-valerate, and therefore should the latter be individually mentioned in the G.R.A.S. list. However, it is NOT mentioned specifically.

Prod. by direct esterification of Citronellol with *iso*-Valeric acid under azeotropic conditions, using a catalyst-starter.

4-34; 33-934; 90-275; 5-238;

## 696: CITRONELLYL VINYL ETHER



$C_{12}H_{22}O = 182.31$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

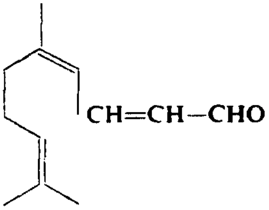
Green-foliage-like, Rose-Geranium type, fresh and rather powerful odor of modest tenacity.

Useful in Citrus cologne types, soap perfumes (as a diffusive and refreshing topnote ingredient), as a supporting item for Geranium notes, etc.

Prod.: from Citronellol plus Acetylene and a catalyst under pressure.

## 697: CITRYLIDENE ACETALDEHYDE

*2*,*6*-Dimethyl-*2*,*6*,*8*-decatrien-*10*-al.
"Muguet aldehyde" (see also Citronellyl oxyacetaldehyde).



$C_{12}H_{18}O = 178.28$

Almost colorless or pale straw-colored oily liquid. Sp.Gr. 0.93. B.P. 247° C. Insoluble in water, soluble in alcohol and oils.

Fresh-herbaceous, Bergamot- and Pear-like odor, also reminiscent of Lemon and Rose. Good tenacity.

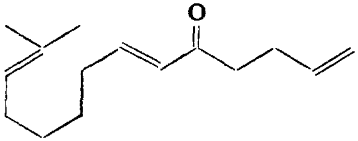
Suggested for use in Muguet, Freesia, Lily, Peony, Verbena and other delicate or fresh-floral compositions.

Prod. by condensation of Citral with Acetaldehyde plus a catalyst.

4-34; 5-97; 86-34;

## 698: CITRYLIDENE ALLYLACETONE

Pseudo-allyl-*alpha*-ionone.



$C_{16}H_{24}O = 232.37$

Pale straw-colored oily liquid.

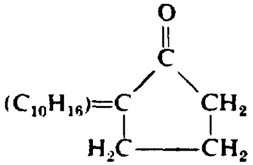
Insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous-fruity, somewhat gassy odor.

This material has little interest as such to the creative perfumer, but it forms an intermediate in the manufacture of an important Ionone-derivative.

Prod.: by condensation of Citral with Allyl methyl ketone. This is the first step in the conventional synthesis of Allyl Ionone.

## 699: alpha-CITRYLIDENE CYCLOPENTANONE



$C_{15}H_{22}O = 218.34$

Pale straw-colored or almost water-white oily liquid.

Powerful, yet light and fruity-floral odor with a peculiar "breadlike" undertone, somewhat limiting the versatility of usage for this chemical.

It can introduce interesting notes in floral bases, including Jasmin, Gardenia, Magnolia, etc., but it is not offered commercially under its proper chemical name, as far as the author knows.

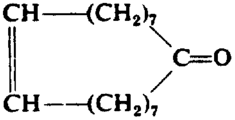
Prod.: By condensation of Citral with Cyclopentanone, according to an (expired) American Patent.

A great number of condensation products using Cyclopentanone as the ketonic component, and various alifatic aldehydes as the aldehydic component have been developed since the late 1930's, but only a few have become commonly marketed.

(See also: 31-85);

## 700: CIVETTONE

*alpha-trans*-Civettone.
Cycloheptadecen-*9*-one-*1*.
Civettone, synthetic (natural C. is *cis*-isomer).



$C_{17}H_{30}O = 250.43$

White or colorless crystalline mass, melting at 32° C. Sp.Gr. (liquid) 0.92. B.P. 344° C.

Almost insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Delicately sweet-animal, rather musky odor, more musky than Exaltone, but not in any way repulsive or unpleasantly animal. Extremely tenacious.

A very useful fixative in Chypres, Oriental fragrance types, Citrus colognes and in many types of floral compositions, particularly those where Rose is a major component.

Civettone introduces excellent skin retention of the fragrance provided the composition is otherwise balanced and completed. In other words, Civettone is not the key with which any mediocre composition becomes a luxury fragrance, but it may be the highly desirable, final touch to many types of nearly completed fragrances.

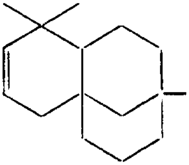
Prod.: Synthetic (several methods), e.g.:

1) via Di-ketenes.
2) via Methylesters of unsaturated dicarboxylic acids.
3) from Aleuretic acid (Hunsdiecker's synthesis).
4) by oxidation of Civettol extracted from Civet.

The *trans*-isomer can be converted to *cis*-isomer via the Ketal.

4-35; 5-187; 5-331; 31-104; 31-282; 31-287; 31-296; 31-312; 30-270ff; 67-278; 156-251; 100-267;
Firmenich's catalogue and datasheet;

## 701: CLOVENE



$C_{15}H_{24} = 204.36$

Colorless oily, slightly viscous liquid.
Sp.Gr. 0.93. B.P. 261-263° C.

Insoluble in water, soluble in alcohol and oils.

Dry-woody, spicy odor, remotely reminiscent of Ambra (the dry notes) and Leather. Good tenacity.

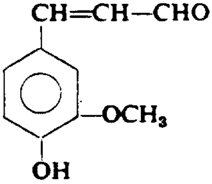
Suggested for use as a blender-fixative in Men's fragrances of the Leather and Ambre-type, in Citrus-colognes, Lavender-Citrus types, and in certain types of women's fragrances, where very dry notes are desirable, e. g. along with Galbanum, Oakmoss, Vetiver acetate, "gamma" Methylionone, etc.

Prod.: by dehydration of *beta*-Caryophyllene alcohol, which is obtained from Clove-Caryophyllenes by cyclization with mineral acid.

67-655; 67-659; 87-322;

## 702: para-CONIFERALDEHYDE

Ferulaldehyde.
"Hadromal".
"Maple aldehyde".
Coniferaldehyde.
*4*-Hydroxy-*3*-methoxy cinnamic aldehyde.



$C_{10}H_{10}O_3 = 178.19$

Colorless crystals. M.P. 83° C.

Soluble in water, alcohol, glycerin, Propylene glycol. Aqueous solutions are often of yellowish color.

Alkaline solutions are yellow if pH is higher than 7.6 but colorless at lower pH.

Sweet-balsamic, pleasantly phenolic-spicy odor, somewhat reminiscent of the odor often encountered in "old" *iso*-Eugenol. Also described as having an unmistakingly Maple-like odor, caramellic-sweet.

Sweet caramellic, Maple-like taste in aqueous media or in milk.

Suggested for use in flavor compositions, particularly in imitation Maple, Vanilla, etc. and in all types of Caramel, Butterscotch, Treacle, Butter-Rum, etc.

Prod.: from Coniferyl alcohol (see next) obtained from the natural glycoside Coniferin (=Laricin=Abietin).

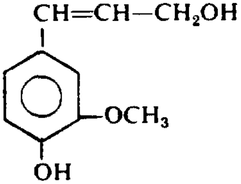
Synthesis from Vanillin is suggested in the literature (with Acetaldehyde in alkaline solution).

NOTE: Among many unavailable or poorly available synthetic flavor materials, Coniferaldehyde is probably one of the most intriguing and interesting. It has only recently been identified in Nature, but may be quite common at very low concentrations in many natural food products. The aldehyde has been known to chemists for more than 70 years.

3-259; 68-986; 58-March, page 52; 60-May, page 60; 104-399; 156-351; 90-515;
See also notes under Coniferyl alcohol.

## 703: CONIFERYL ALCOHOL

*gamma*-Hydroxy-*iso*-Eugenol.
Ferula alcohol.
*3*-(*4*-Hydroxy-*3*-methoxyphenyl)-*2*-propen-*1*-ol.
*4*-Hydroxy-*3*-methoxy cinnamic alcohol.
Lubanol.



$C_{10}H_{12}O_3 = 180.21$

White (colorless) crystals. M.P. 74° C.

Very slightly soluble in water, soluble in alcohol and oils.

Polymerizes with weak mineral acids and certain organic acids, turning into an amorphous, odorless gum.

This chemical could find extensive use as a fixative and blender in various types of floral, balsamic and Oriental fragrances. However, it is not generally available in the state of chemical or olfactory purity desirable to the perfumer.

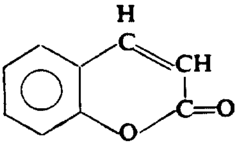
The alcohol and its esters occur in very large amounts in Nature e. g. Siam Benzoin (total about 78% crystalline and amorphous alcohol and esters), in the barks of various Lonicera species (Honeysuckle), Acer species (Maple), Scorzonera roots and rhizomes, Asparagus, Styrax tonkinense, Asafoetida, Sugar beets, etc.

Prod.: by enzymatic hydrolysis of the glucoside Coniferin (= Abietin). Also as a breakdown product of naturally occurring Lignin, the structure of which is not completely clear. The three major breakdown products are: *para*-Hydroxycinnamic alcohol (oxidizes to *para*-Hydroxybenzaldehyde, precursor of "Raspberry ketone"), Coniferyl alcohol (oxidizes to Coniferaldehyde and Vanillin) and Sinapyl alcohol, which oxidizes to Syringa aldehyde.

1-440; 100-282; 68-982; 104-89; 104-91; 104-399; 124-145; 124-150; 130-447;
Also: R. Hegnauer: Chemotaxonomie der Pflanzen (1962). "Canadian Journal of Biochemistry and Physiology", 25 (1959) vol. 37.

## 704: COUMARIN

*cis-ortho*-Coumaric acid anhydride.
*1,2*-Benzopyrone.
*5,6*-Benzo-*alpha*-pyrone.
"Tonka Camphor".
*ortho*-Hydroxycinnamic acid, lactone.



$C_9H_6O_2 = 146.15$

White crystals, crystalline powder, leaflets or rhomboid crystals. M.P. 68° C.

B.P. 291° C.

Sublimes, but is hardly volatile with steam, except with superheated steam.

Soluble 0.3 % in water, 8 % in alcohol, freely in most perfume oils.

Sweet, herbaceous-warm, somewhat spicy odor, in extreme dilution more haylike, nutlike, tobacco-like.

Bitter taste, except when highly diluted, then sweet-herbaceous, haylike, nutlike.

Extensively used in perfumery to support herbaceous odors, Lavender, Lavandin, Rosemary, Citrus oils, Oakmoss, etc., and as a fixative in numerous types of fragrances. Almost a standard ingredient in Fougère types with Amylsalicylate and Lavender-notes, with or without Oakmoss.

A classical masking agent for Iodoform odor, Phenolic odors, Quinoline odors, etc.

NOTE: Not permitted for food use in the U.S.A. Also banned from food flavorings in a number of other countries. However, extracts of certain botanical materials, rich in Coumarin, are still in use as Tobacco flavoring agents and in other flavors.

The hazardous level of Coumarin is estimated at 3 grams per day for adult human beings.

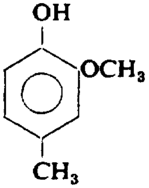
Prod.:

1) from Salicylic aldehyde + Acetic anhydride + anhydrous Sodium acetate.
2) from *ortho*-Cresol + Carbonyl chloride, followed by chlorination of the resulting Carbonate, fusion of the Dichlorocresol carbonate with Alkali acetate and Acetic anhydride plus a catalyst.

1-544; 5-209; 26-466; 30-256; 31-165; 85-53; 90-591; 100-292; 103-298; 106-120; 1ff56-131; B-XVII-328; 4-36; 86-35; 96-177; 95-191;

## 705: CREOSOL

*4*-Methyl guaiacol.
*2*-Methoxy-*4*-methylphenol.
*1*-Hydroxy-*2*-methoxy-*4*-methylbenzol.
*2*-Methoxy-*para*-cresol.
Homocatechol monomethylether.



$C_8H_{10}O_2 = 138.19$

Viscous, yeelowish oil, solidifying in the cold. The prismatic crystals melt at 6° C.

Sp.Gr. 1.10. B.P. 222° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-spicy, phenolic-leathery odor with distinctly Vanilla-like undertones, balsamic-warm sweetness, but overall too medicinal to become classified as a versatile, floral-balsamic ingredient.

Excellent additive and modifier in artificial Ylang-Ylang, Cassie-bases, Jasmin bases, Lily, Gardenia, etc.

Finds use in flavor compositions for imitation Vanilla, Clove, various fruit compositions, Rum flavors, etc. and in Nut-Nougat flavor bases.

Concentration will be about 0.02 to 1 ppm. in the finished consumer product. In beverages, however, it may be as high as 10 to 20 ppm.

Prod. by hydrogenation of Vanillin in the presence of a catalyst.

G.R.A.S. F.E.M.A. No.2671.

26-466; 68-469; 72-67; 90-383; B-VI-878;

## 706: CREOSOTE

Beechwood Creosote.

A mixture of phenols from the tar obtained by destructive distillation of Beechwood.

The main components are: Guaiacol and Creosol (see these monographs).

Colorless or pale yellowish oily liquid.

Sp.Gr. 1.08.

Powerful and penetrating odor, resembling that of smoke (from wood).

0.5% soluble in water, miscible with alcohol and oils. Soluble in Glycerin and Propylene glycol.

Burning taste and mouthfeel.

Occasionally used in perfumery, e. g. to introduce certain desirable notes in Oakmoss bases, wood odors, Leather fragrance, etc.

Used in flavor compositions for its "smoky" effect, simulating the flavor of smokehouse-treated meats, etc., for certain seafood flavors, etc.

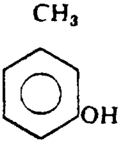
G.R.A.S.

Prod.: Wood tar from Beechwood is redistilled. The heavier-than-water layer is treated with Sodium carbonate and distilled again. From this distillation the heavier-than-water layer is subsequently treated with Potassium hydroxide, and then with Sulfuric acid. Finally it is redistilled at atmospheric pressure. The distillate coming over at 200 to 220° C. is collected and classified as "Creosote".

100-1105; 124-233;

## 707: meta-CRESOL

*3*-Hydroxytoluene.
*3*-Cresol.
*1*-Methyl-*3*-hydroxybenzene.
*meta*-Methylphenol.



$C_7H_8O = 108.14$

Colorless liquid. Sp.Gr. 1.03. M.P. 12° C. B.P. 203° C.

Solidifies in the cold. Volatile with steam.

Soluble 2% in water, soluble in alcohol and oils.

Dry-tarry, medicinal-leathery odor, conventionally described as "phenolic".

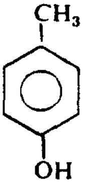
Useful as a floralizing companion to Indole in sharp-exotic flower fragrances, Lily (Bermuda-lily, etc.), Narcisse, etc. Concentration in the perfume composition will usually be about 0.1%, sometimes slightly higher, mostly lower than 0.1%.

Prod.: from Coal tar cresolic mixture, by fractionated distillation. - Or by reduction of *meta*-Hydroxybenzaldehyde.

26-466; 68-419; 90-370; B-VI-373;

## 708: para-CRESOL

*4*-Hydroxytoluene.
*1*-Methyl-*4*-hydroxybenzene.
*para*-Methylphenol.



$C_7H_8O = 108.14$

White crystals, melting at 35° C. B.P. 202° C.

Sp.Gr. 1.03.

Soluble 1.8% in water, readily soluble in alcohol and perfume oils, Propylene glycol, soluble in Glycerin.

Tarry-smoky, medicinal ("phenolic") type odor. Strongest of the *3* isomers. In extreme dilution sweeter, almost floral, less leathery than *meta*-Cresol.

Useful in trace amounts as a floralizer for Narcissus and Lily type perfumes and bases. More recently used in "medicated" type soaps, partly as an odorant, partly for its bactericidal effect. Also used for artificial Ylang-Ylang and other floral bases. Finds some use in flavor compositions, applied in trace amounts in imitation Vanilla, in Nut flavors, etc.

G.R.A.S. F.E.M.A. No.2337.

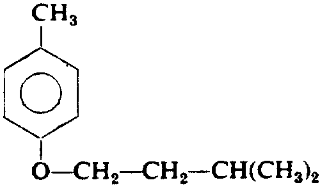
Prod.:

1) by Alkali fusion of *para*-Toluene sulfonic acid.
2) from *para*-Toluidine.

2-163; 7-145; 30-238; 31-23; 26-446; 68-420; 90-373; 1-437; B-VI-389.

## 709: para-**CRESOL AMYLETHER**

"Amyl cresyl oxide".
*para*-Cresol-*iso*-amylether.



$C_{12}H_{18}O = 178.28$

Colorless liquid. B.P. 242° C. Sp.Gr. 0.96.

Almost insoluble in water, soluble in alcohol and perfume oils.

Floral-herbaceous, Cananga-like odor with a green undertone.

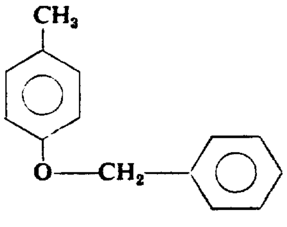
Useful in Hyacinth, Narcissus, Lily, Gardenia, etc. Occasionally used in Jasmin bases.

Prod. from *iso*-Amylbromide plus *para*-Cresolsodium in aqueous solution.

37-172;

## 710: para-**CRESOL BENZYLETHER**

Benzyl-*para*-cresylether.
"Benzyl cresyl oxide".
"Jasmin oxide".



$C_{14}H_{14}O = 198.27$

White crystals. M.P. 42° C. B.P. 325° C.

Almost insoluble in water, soluble in alcohol and perfume oils.

Heavy-floral, rather pungent, Jasmin-like odor.

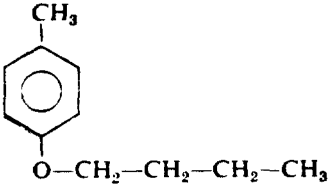
Useful in low-cost Jasmin fragrances, where alkali-stability and power call for special ingredients.

Prod.: from Benzyl chloride + *para*-Cresol sodium in aqueous solution.

4-21; 37-171; 37-172; 86-35;

## **711:** para-**CRESOL**-n-**BUTYLETHER**

"Cresyl butyl oxide".
"Cananga ether" (this term also used for *para*-Cresol methylether).



$C_{11}H_{16}O = 164.25$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.
B.P. 220° C. Sp.Gr. 0.98.

Heavy-floral, but rather soft and sweet odor, much less pungent than that of the -ethylether, also more tenacious. More woody undertone.

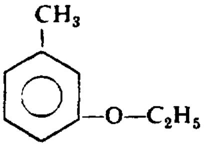
Useful in Cananga compositions, various heavy floral bases, Narcisse, Lily, Gardenia, Jasmin, etc.

Prod.: from *para*-Cresolsodium and *n*-Butylbromide.

4-35; 31-146; 37-172; 86-35;

## **712:** meta-**CRESOL ETHYL ETHER**

*meta*-Ethoxy toluene.
*meta*-Tolylether.



$C_9H_{12}O = 136.20$

Colorless liquid. Sp.Gr. 0.96. B.P. 192° C.

Insoluble in water, soluble in alcohol and perfume oils.

Pungent-floral, sweet and heavy odor of leathery Cananga type.

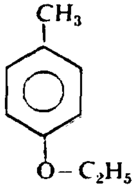
Very rarely used in perfumery, and not a common commercial item.

Prod.: from *meta*-Cresol in weak alkaline solution (aqueous) with Diethyl sulfate.

26-550; B-VI-376;

## **713:** para-**CRESOL ETHYL ETHER**

*4*-Ethoxy-*1*-methyl benzol.
(Ethyl)-*para*-Tolylether.
(Ethyl)-*para*-Cresylether.
Ethyl-*para*-cresylate.



$C_9H_{12}O = 136.20$

Colorless liquid. Sp.Gr. 0.97. B.P. 189° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, pungent-floral, deep-sweet, warm odor, suggestive of Ylang-Ylang, Pandanus and other exotic flowers.

Useful in perfume compositions of the heavy-floral type, in artificial Ylang-Ylang, in various types of soap perfume and, in general as a floralizer with considerable power.

Its comparatively high vapor pressure causes some problems in suitable fixation and puts a limit to a practical use-concentration. Only in veritable Ylang-reproductions is it possible to use about 5% or more, while normally the ether is used at 1 to 2% in the perfume composition.

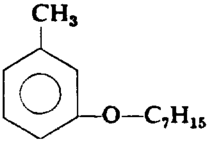
It is somewhat softer than the Methyl ether and not as violently harsh, but it is also less Ylang-Ylang-like than the Methyl ether, mainly because it has a peculiar nut-like, or earthy undertone, typical of many Phenolethylethers.

Prod.: from *para*-Cresol in diluted aqueous alkaline solution with Diethyl sulfate at about 30° reaction temp. followed by heating and steamdistillation of the resulting ether.

4-35; 4-110; 26-550; 86-35; 156-141; B-VI-393; 95-115;

## **714:** meta-**CRESOL HEPTYLETHER**

*meta*-Cresol heptyloxide.



$C_{14}H_{22}O = 206.23$

Colorless liquid. Insoluble in water. Soluble in alcohol and oils. Sp.Gr. 0.91. B.P. 260° C.

Peculiar metallic-green, smoky odor with oily-herbaceous undertones, remotely reminiscent of Lily flowers.

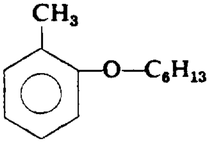
Occasionally used in Jasmin bases, Narcisse and Lily, mainly to introduce oily-herbaceous notes.

Prod.: from *meta*-Cresolsodium and *n*-Heptyliodide in aqueous solution.

4-86;

## **715:** ortho-**CRESOL HEXYLETHER**

*ortho*-Cresol-*n*-hexyloxide.



$C_{13}H_{20}O = 192.30$

Colorless liquid, insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.91. B.P. 253° C.

Sweet, almost balsamic-herbaceous, slightly medicinal odor, resembling the odor of Salol (Phenyl salicylate). Good tenacity.

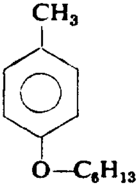
Very rarely used in perfumery. Could find some use in heavy floral bases, Jasmin, Narcisse, Gardenia, etc. but does not offer any unusual notes or effects.

Prod.: from *ortho*-Cresol sodium + *n*-Hexylbromide in aqueous solution.

4-109; 86-35;

## **716:** para-**CRESOL HEXYLETHER**

*para*-Cresyl-*n*-hexyl oxide.



$C_{13}H_{20}O = 192.30$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol. B.P. 245° C. Sp.Gr. 0.92.

Somewhat dry-metallic, green, Narcissus-like, odor, sharper than that of the *ortho*-ether, and less herbaceous.

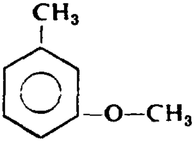
Has been suggested for use in floral perfume bases, such as Lily, Jasmin, Narcissus, etc. but this ether does not seem to offer any unusual or very special notes to such creations. It is very rarely offered commercially.

Prod.: from *para*-Cresol sodium plus *n*-Hexylbromide in aqueous solution.

4-110; 86-35;

## 717: meta-CRESOL METHYLETHER

*3*-Methoxy-*1*-methyl benzene.
Methyl-*meta*-tolyl ether.



$C_8H_{10}O = 122.17$

Colorless liquid. Almost insoluble in water, soluble in alcohol and perfume oils.
Sp.Gr. 0.97. B.P. 177° C.

Although this ether has an overall floral fragrance, it is more earthy, and much less sweet than the *para*-ether. Pungent, semi-dry, nut-like, almost mossy odor.

This ether blends excellently with Oakmoss products in which it will emphasize the earthy-nut-like notes, but it can also support the floral notes in Cananga and Ylang-Ylang bases. Interesting in leather-like fragrance types.

Occasionally used in flavor compositions for its Hazelnut-like character, prominent in its taste in aqueous or oily media.

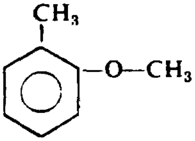
Prod.: from *meta*-Cresol and Sodium hydroxide in weak aqueous solution with Dimethyl sulfate.

NOTE: It is interesting to note that this ether has a Hazelnut-like fragrance and aroma, being closely related (chemically) to Resorcinol dimethylether, classical Hazelnut-item.

4-86; 26-612; B-VI-376; 96-226;

## 718: ortho-CRESOL METHYLETHER

*ortho*-Methyl anisole.
Methyl-*ortho*-tolylether.
*ortho*-Methoxy toluene.



$C_8H_{10}O = 122.17$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.98. B.P. 172° C.

Pungent-floral, warm, but almost "gassy" (undiluted) odor with earthy-Walnut-like undertones.

In proper dilution (about 1:300,000) it has a pleasant, sweet, fruity-nutlike flavor.

Occasionally used in perfume compositions as a modifier in heavy floral bases, Cananga, Ylang-Ylang, etc.

Finds some use in flavor compositions, particularly those of the "Fruit-and Nut" type.

The concentration in the finished consumer product will usually be about 1 to 4 ppm.

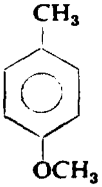
G.R.A.S. F.E.M.A. No.2680.

Prod.: from *ortho*-Cresol in weak aqueous alkali solution with Dimethylsulfate.

26-612; B-VI-352;

## 719: para-CRESOL METHYLETHER

Methyl-*para*-cresol.
Methyl-*para*-cresylate.
*4*-Methoxy-*1*-methyl benzene.
Methyl-*para*-tolylether.
*para*-Methyl anisole.
*para*-Methoxy toluene.
"Canangol".



$C_8H_{10}O = 122.17$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils. Sp.Gr. 0.97. B.P. 176° C.

This is the most commonly used of all the Cresolethers.

Pungent, sharp-sweet odor when undiluted, Hyacinth-Wallflower-Ylang type odor when modestly diluted (concentrations below 5-6% in perfume composition), greener and more fruity when highly diluted, almost Marigold like.

Useful for above floral notes, for Jasmin, Lilac, Broom, and in general to introduce powerful floral notes at low cost. This ether performs well in soap.

Finds some use in flavor compositions, mainly in imitation Nut, Black Walnut, Walnut, Maple, Spice blends and certain Berry type flavors.

Concentration will be about 0.5 to 8 ppm. in the finished product.

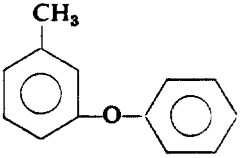
Prod.: from *para*-Cresol sodium and Dimethyl sulfate in aqueous solution.

G.R.A.S. F.E.M.A. No.2681.

4-110; 5-219; 26-612; 31-146; 34-679; 37-172; 68-426; 86-35; 90-382; 106-245; 156-141; B-VI-392;

## 720: meta-**CRESOL PHENYLETHER**

Phenyl-*meta*-cresyl oxide.



$C_{13}H_{12}O = 184.24$

Colorless liquid, solidifying in the cold. B.P. 276° C.

Insoluble in water, soluble in alcohol, miscible with perfume oils.

Somewhat harsh-metallic, Geranium-like odor of good tenacity.

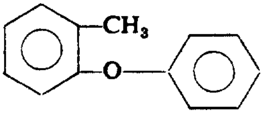
Very rarely used in perfumery, seldom offered commercially.

Prod. by heating *meta*-Chlorotoluene with Chlorobenzene and aqueous alkali under pressure to about 300° C.

95-115;

## 721: ortho-**CRESOL PHENYLETHER**

Phenyl-*ortho*-tolylether.



$C_{13}H_{12}O = 184.24$

Colorless liquid, solidifying in the cold, melting at 22° C. B.P. 269° C.

Insoluble in water, soluble in alcohol and oils.

Somewhat harsh-green, metallic, Geranium-like odor, reminiscent of the odor of Diphenyl oxide.

Used to be quite popular in soap perfumery, but has lost its importance since it does not contribute any unusual notes or outstanding power.

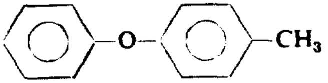
Prod.:

1) from Bromobenzene by heating to 200° C. with Potassium hydroxide and Copper.
2) from *ortho*-Chlorotoluene and Chlorobenzene by heating with aqueous alkali under pressure to 300° C.

95-115;

## 722: para-CRESOL PHENYLETHER

"Cresyl phenyl oxide".
Phenyl cresyl ether.
Phenyl-*para*-tolylether.



$C_{13}H_{12}O = 184.24$

Colorless liquid, insoluble in water, soluble in alcohol, miscible with oils. B.P. 278° C. Sp.Gr. 1.06.

Powerful, heavy-floral, somewhat green and sharp odor, reminiscent of Narcisse, Rose and Orangeblossom.

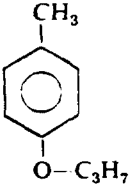
Useful in perfume compositions of the named odor types, stable in alkali and mild acid media. It is quite tenacious and will partly act as a fixative. However, it must be well blended with milder smelling fixatives in order not to "stick out" in the later stages of evaporation of the perfume composition.

Prod.: from *para*-Chlorotoluene and Chlorobenzene by heating under pressure with aqueous alkali.

4-111; 7-146; 7-337; 86-35; 156-142; 37-172; 95-115; 163-63;

## 723: para-CRESOL PROPYL ETHER

*1*-Methyl-*4*-propoxy benzene.
NOTE: Do NOT confuse with *para*-Propyl anisole (= Dihydro anethole).



$C_{10}H_{14}O = 150.22$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 205° C. Sp.Gr. 1.01.

Pungent, sweet-herbaceous, slightly floral odor, remotely reminiscent of Lily and Narcissus, however, mainly anisic in type.

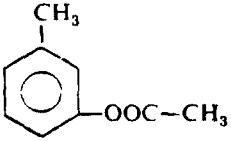
Occasionally used in perfumery, mainly for its power, stability in alkali, and for its low cost (in proportion to odor effect).

Prod.: from *para*-Cresol sodium in aqueous solution with *n*-Propyl iodide.

34-679; 37-172; 86-35;

## 724: meta-CRESYL ACETATE

Acetyl-*meta*-cresol.
"Cresatin".



$C_9H_{10}O_2 = 150.18$

Colorless liquid. Slightly soluble in water, soluble in hot water, in alcohol and oils. B.P. 212° C.

Powerful and pungent-floral odor of Narcissus-Ylang-Ylang type – sharper than the Cresyl ethers, but also fresher and more penetrating. Some observers find an animal note in this odor.

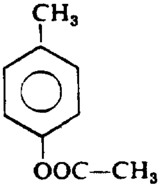
Occasionally used in perfume compositions of above floral types, or, in general, as a powerful floral additive at low cost.

Prod.: by Acetylation of *meta*-Cresol with Acetic anhydride.

26-466; 35-35; 61-72; B-VI-379;

## 725: para-CRESYL ACETATE

Acetyl-*para*-cresol.
"Narceol".
*para*-Tolyl acetate (name also used for *para*-Methyl benzyl acetate).



$C_9H_{10}O_2 = 150.18$

Colorless liquid, volatile with steam. Poorly soluble in water, miscible with alcohol and oils, soluble in Propylene glycol. Sp.Gr. 1.05. B.P. 212° C.

Pungent Lily-like odor, penetrating, floral, Narcissus-like in high dilution, Horse-like, urine-like undertones in higher concentration. Pleasant notes are obtained normally at concentrations below 1 % in the perfume creation, but the material is still capable of totally ruining a composition when the acetate is applied in combination with certain fragrance notes or single chemicals.

Finds some use in flavor compositions for its intensely floral power, which can support fruity notes, nut-like aromas, etc.

The concentration in the finished product is usually about 0.5 to 10 ppm, but may reach 220 ppm in chewing gums.

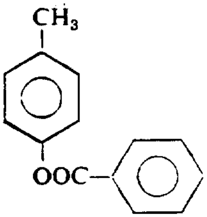
Prod.: by Acetylation of *para*-Cresol.

G.R.A.S. F.E.M.A. No.3073.

35-35; 43-500; 86-34; 106-121; 156-143;

## 726: para-CRESYL BENZOATE

*para*-Tolyl benzoate. (so-called).



$C_{14}H_{12}O_2 = 212.25$

Colorless or white plate crystals.

M.P. 72° C. B.P. 316° C.

Insoluble in water, modestly soluble in alcohol, miscible with most perfume oils.

Very faint odor, somewhat sweeter than that of *para*-Cresylsalicylate, more floral.

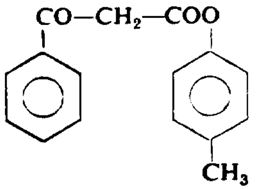
Rarely used in perfumes, occasionally as a fixative-modifier in Lily-Jasmin-Narcissus type bases.

Prod.: from *para*-Cresol sodium and Benzoyl chloride.

26-696; B-IX-120;

## 727: para-CRESYL BENZOYL ACETATE

*para*-Tolyl benzoylacetate.



$C_{16}H_{14}O_3 = 254.29$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Herbaceous-sweet, yet somewhat pungent and very tenacious, floral-green odor with resemblance to Narcissus and with pleasant, balsamic, Ambre-Labdanum-like undertones.

It has the pungency of the cresylic ethers in a pleasantly modified and subdued version, and without the medicinal undertones of the conventional cresylic ethers or esters.

A very useful item in Narcissus bases, Lily, Gardenia and Tuberose. Blends excellently with refined Styrax products, Ambrain-products, etc.

The material is rarely offered under its proper chemical name, but it has established itself in a number of successful bases and specialties, and it is relatively inexpensive in production. Only because Lily and Narcisse are not extremely popular fragrance types, and their role in complex fragrances will always be a minor one, the title material will probably remain unknown or unavailable to most perfume houses, and not come into strong demand by the industry.

Prod.: from Ethyl benzoyl acetate and *para*-Cresol by Trans-esterification in the presence of Phosphorous oxychloride.

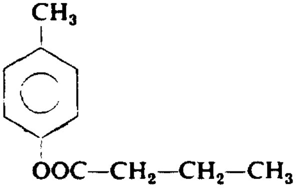
Other methods include the condensation of *para*-Cresylacetate with Ethylbenzoate with a Sodium type condensing agent, and the treatment of Benzoyl acetylchloride with Sodium-*para*-cresol.

68-938;

## 728: para-**CRESYL BUTYRATE**

*para*-Tolyl-*n*-butyrate (somewhat confusing name).

NOTE: The *iso*-Butyrate is the most common commercial product (see next).



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

B.P. 244° C.

Narcissus-like odor, softer and fruitier than that of the Acetate, and not at all "urine-like" in its undertones.

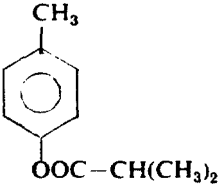
A comparatively rare chemical, occasionally used for Ylang-Ylang bases, Narcissus, etc.

Prod.: from *para*-Cresol and *n*-Butyric acid, using Phosphoroxychloride as a catalyst.

4-35; 86-35;

## 729: para-**CRESYL**-iso-**BUTYRATE**

*para*-Tolyl-*iso*-butyrate (somewhat confusing name).



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid, insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.00.

B.P. 237° C.

Pronounced Lily-Narcissus-like odor, somewhat pungent and intense, but in proper dilution pleasant floral-oily-green Lily-Ylang-like.

Useful in perfume compositions at concentrations around 0.5% when well blended with milder floral components and sweet fixatives. Also as a modifier for *para*-Cresyl caprylate in waxy-herbaceous floral bases.

Finds some use in fruit flavor compositions. The concentration in the finished product is usually about 0.05 up to 8 ppm in rare cases.

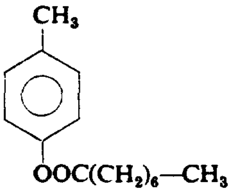
G.R.A.S. F.E.M.A. No.3075.

Prod.: from *para*-Cresol and *iso*-Butyric acid using Phosphoroxychloride as a catalyst.

4-26; 33-732; 156-143;

## 730: para-CRESYL CAPRYLATE

*para*-Tolyl octoate.
*para*-Cresyl octoate.
*para*-Tolyl octanoate.
*para*-Cresyl octylate.
"Narcissin K".



$C_{15}H_{22}O_2 = 234.34$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.
Sp.Gr. 1.00. B.P. 265° C.

Floral and somewhat indolic, Narcisse-like odor with soft and oily-herbaceous undertones, good tenacity. There are great variations in the odor picture of products from different manufacturers, and mere traces of one or the other parent component can completely change an odor description of the material.

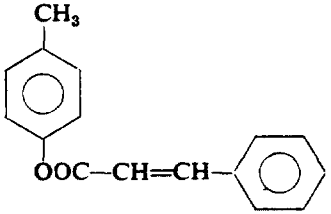
Very useful in floral perfume bases, where green-herbaceous, mild og oily undertones should accompany the distinctly floral notes. Blends well with Indole, with Rose bases, Jasmin bases, Lily, Hyacinth and Narcissus, etc.

The odor effect is persistent yet very discrete, provided the ester is free from Caprylic acid, and free from Cresol.

Prod. from *para*-Cresol and Octanoic acid, using Phosphoroxychloride as a catalyst.

4-35; 4-110; 35-404; 86-35;

## 731: para-CRESYL CINNAMATE



$C_{16}H_{14}O_2 = 238.29$

White crystals. Insoluble in water, soluble in alcohol, miscible with most perfume oils.

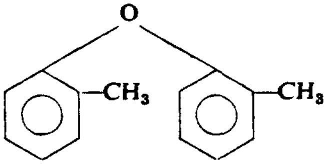
Very faint, delicately floral, sweet odor of considerable tenacity. Overall Lily-like, but mild enough to become a fixative background of other floral types, Oriental fragrances, etc.

Very rarely offered commercially, rarely used.

Prod.: from *para*-Cresolsodium in aqueous solution with Cinnamyl chloride in presence of a catalyst.

## 732: ortho-CRESYL ETHER

*ortho*-Cresyl oxide.



$C_{14}H_{14}O = 198.27$

White crystals. Almost insoluble in water, soluble in alcohol and oils.

Metallic-green, Geranium-like, moderately tenacious odor, somewhat resembling that of Diphenyloxide, yet slightly sweeter, less "cool".

Very rarely used in perfumery. Only occasionally offered commercially.

Prod.:

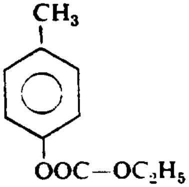
1) from *ortho*-Cresol heated over Thorium at 500° C.
2) from Bromotoluene and Potassium phenoxide heated with Copper powder catalyst at 220° C.

7-147; 31-146;

Sometimes confused with *ortho*-Ethoxy toluene.

Commercial Di-tolyl ether is primarily *para*-Tolyl ether. See Di-tolyl ether.

## 733: para-CRESYL ETHYLCARBONATE



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

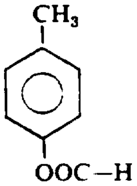
Sweet, rather powerful floral, Narcissus-like odor of modest tenacity. The chacteristic difference between this material and the conventional Cananga-Narcisse-Lily chemicals lies mainly in the soft sweetness, the power of the ethylcarbonate without harshness, as compared to e. g. the ethylether.

An interesting item in Lily-Ylang and Narcissus bases, however, it requires proper modifiers to become fully attractive.

Rarely, if ever, offered under its proper name, but quite extensively used in certain floral bases, specialties, etc.

Prod.: from *para*-Cresol and Ethyl carbonate by cross-esterification, using Sodium Methylate catalyst.

## 734: para-CRESYL FORMATE



$C_8H_8O_2 = 136.15$

Colorless liquid. Very slightly soluble in water, soluble in alcohols and oils.

Very powerful Lily-Jasmin-Lilac type odor. The herbaceous and green notes are more pronounced in this ester than in the Acetate, and the overall odor impression bears some resemblance to Lilac and Jasmin.

The dry undertone is also characteristic of this ester.

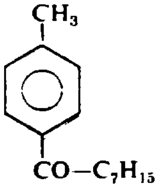
An interesting item for Hyacinth and Lilac, e. g. as a modifier for Benzyl formate.

Prod. from *para*-Cresol and Formic acid (or Formacetic acid mixture) using Acetic anhydride or Mineral acid catalyst.

4-35;

## 735: para-CRESYL HEPTYL KETONE

*para*-Caproyltoluene.



$C_{15}H_{22}O = 218.34$

Colorless oily liquid, solidifying in the cold.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet-herbaceous, slightly green and oily odor with variable amounts of cresylic notes, most conceivably derived from impurities (decomposition ?).

This ketone, rarely offered under its proper name and not often brought to the perfume chemical market, has been used in perfume compositions of the heavy-floral type, also in Violet and Narcisse bases. It blends well with the Ionones and other Violet materials, with Vetiver and Oakmoss, and with many floral chemicals, too.

The ketone was introduced many decades ago by Agfa (Germany) and has fallen into oblivion among modern perfumers. It may still be used in certain specialties, but is rarely found on the shelf in a perfume laboratory.

Prod.:

1) by oxidation of *para*-Octyl toluene.
2) from *para*-Cresyl octoate by heating with Aluminium chloride in a so-called Fries' rearrangement.

33-158;

## 736: CRESYLIC ACID

"Coal tar Creosote".

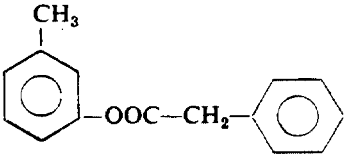
The commercial product is a composite of fractions of Cresylic acids (Coal tar phenols), boiling at 205° C. and upwards. (Atmospheric pressure).

See also CREOSOTE. (Beechwood Creosote).

100-295; 124-233;

## 737: meta-CRESYL PHENYLACETATE

*1,3*-Tolyl phenylacetate.



$C_{15}H_{14}O_2 = 226.28$

White granular crystals, melting at 51° C. Insoluble in water, soluble 15% in alcohol, miscible with most perfume oils.

Lily-Narcissus-YlangYlang type odor.

More musky, and also milder than the *para*-Cresyl phenylacetate, but produces very "chemical" overtones slightly beyond normal use-level.

Useful in Honey-bases, and in Jasmin, Lilac, Narcissus bases, etc.

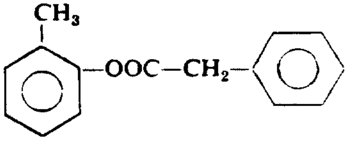
Concentration in perfume compositions will normally be well below 1%, but may come higher in bases.

Prod. from *meta*-Cresol sodium plus Phenyl acetylchloride.

4-36; 34-246; 106-123;

## 738: ortho-CRESYL PHENYLACETATE

*1,2*-Tolyl phenylacetate.



$C_{15}H_{14}O_2 = 226.28$

White crystals. Insoluble in water, soluble in alcohol, miscible with perfume oils.

M.P. 45° C.

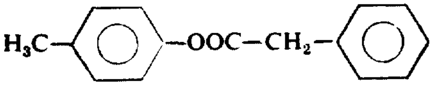
Rarely, if ever, offered commercially. This ester is the rarest and least useful of the three isomers.

Prod.: from *ortho*-Cresolsodium and Phenyl acetylchloride.

4-36;

## 739: para-CRESYL PHENYLACETATE

*para*-Tolyl phenylacetate (confusing name).
"Narceol". (Name also used for other chemicals).
Narcissin.



$C_{15}H_{14}O_2 = 226.28$

White granular crystals. M.P. 75° C.

Insoluble in water, 2.5 % soluble in alcohol, miscible with most perfume oils, poorly soluble in Propylene glycol.

Very tenacious Lily-Hyacinth-Jonquil type odor. The nuances in odor occur when the material is not chemically pure, e. g. from traces of Phenylacetic acid ("Horse-urine" odor) or traces of *para*-Cresol (medicinal odor).

Usually applied at less than 1 % in the perfume composition, this ester should be carefully blended with highboiling or powerful odorants in order to achieve a pleasant effect. It performs well in Jasmin, Tuberose, Gardenia, Lily, Hyacinth, Narcissus and other floral and floral-green bases.

Occasionally used in flavor compositions for imitation Honey, Butter, Nut, Caramel, Fruit, etc.

The concentration in the finished product will usually be about 1 to 6 ppm.

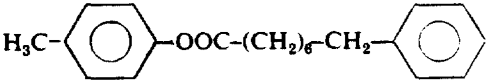
G.R.A.S. F.E.M.A. No.3077.

Prod.: from *para*-Cresol plus Phenylacetic acid with Phosphorpentoxide – or: with Phosphoroxychloride in aqueous alkaline solution.

4-36; 5-272; 34-246; 61-73; 106-124; 103-139; 155-96;

## 740: para-CRESYL PHENYLCAPRYLATE

*para*-Cresyl phenyloctanoate.



$C_{21}H_{26}O_2 = 310.44$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Very faint, sweet-floral odor of considerable tenacity. Reminiscent of Rose and Narcisse with emphasis on the green-woody undertones.

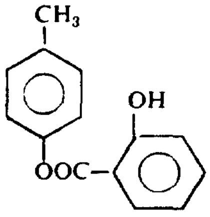
Very rarely used, rarely offered commercially.

Was probably marketed when the *para*-Cresyl octoate and the *para*-Cresyl phenylacetate both became known and rather popular. However, the subject ester has never achieved any great interest among perfumers.

4-36;

## 741: para-CRESYL SALICYLATE

*para*-Cresyl-*ortho*-hydroxybenzoate.



$C_{14}H_{21}O_3 = 228.25$

White rhomboid crystals, melting at 39° C.

Insoluble in water, soluble in alcohol and oils.

Very faint floral-green, tenacious odor, reminiscent of Narcissus, Hyacinth, etc. but more delicate than the conventional *para*-Cresyl esters.

The mildness of this odor is often ruined by the presence of trace amounts of free *para*-Cresol or Phenol.

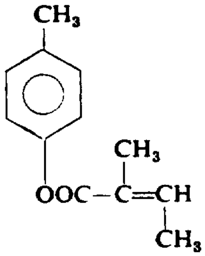
Useful in Narcissus, Jasmin, etc., and blends excellently with Oakmoss products in Chypres, Men's Fougères, etc.

Prod.: from *para*-Cresol with Salicylic acid and Phosphoroxychloride.

26-698; B-X-80;

## **742:** para-**CRESYL TIGLATE**

*para*-Cresyl-*trans-alpha-beta*-dimethylacrylate.



$C_{12}H_{14}O_2 = 190.24$

White crystals. Insoluble in water, soluble in alcohol and oils.

Herbaceous-green, warm and somewhat tobacco-like or honeylike odor, yet not distinctly sweet, rather caramellic.

Good tenacity.

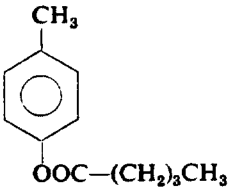
Traces of Cresol or Tiglic acid may easily change this odor picture.

Interesting in Narcissus, Hyacinth, Muguet, Lily, etc.

Traces can impart good notes in certain types of Rose base.

Prod.: from *para*-Cresolsodium and Tiglyl chloride (or Tiglic acid plus Phosphoroxychloride).

## **743:** para-**CRESYL VALERATE**



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Animal-floral odor, sometimes described as musky.

Finds some use as a modifier for Civet products, along with Phenylacetic acid and its derivatives.

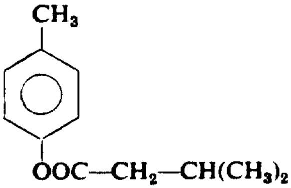
Can give good effects in Rose bases of the "Oriental" type.

Rarely offered commercially.

Prod.: from *para*-Cresol plus *n*-Valeric acid with Phosphoroxychloride.

4-36;

## **744:** para-**CRESYL**-iso-**VALERATE**



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Tobacco-like, animal, sweet-herbaceous odor with undertones resembling Civet.

Useful as a modifier for Civet, Skatole, Phenylacetic acid, etc. in Civet bases and other animal types bases.

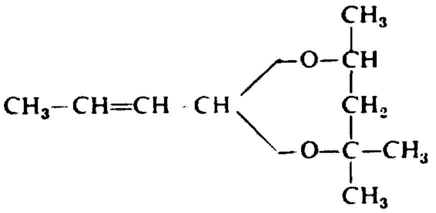
Interesting in the more sophisticated types of Pine fragrances. Can introduce pleasant notes and effects in Rose, Tobacco, Narcissus, Oriental fragrances, etc.

Prod.: from *para*-Cresol and *iso*-Valeric acid with Phosphoroxychloride.

4-36;

# 745: CROTONALDEHYDE-2-METHYLPENTANE-(2,4-DIOL)-ACETAL

*2*-Propenyl-*4,6,6*-trimethyl-*1,3*-dioxane.



$C_{10}H_{18}O_2$ = 170.25

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils. B.P. 190° C.

Soft, floral-green, almost herbaceous-green odor, not unlike the lower "carbinols" (Dimethyl benzyl carbinol, etc.) but overall sharper, lighter, fresher.

Has been suggested for use in perfume compositions as a modifier in modern floral fragrance types.

Prod.: from Croton aldehyde and *2*-Methylpentane-*2,4*-diol by condensation in presence of a catalyst.

# 746: CROTONYL-iso-THIOCYANATE

Crotonyl Mustard oil.
*beta*-Butenyl-*iso*-thiocyanate.
*beta*-Methallyl Mustard oil.

$CH_3—CH=CH—CH_2—N=C=S$
(synthetic material)

$C_5H_7NS$ = 113.19

Colorless liquid. B.P. 160° C.

Almost insoluble in water, soluble in alcohol and oils.

Commercial lots (very rarely offered) are mostly composed of the isomer:

*gamma*-Butenyl-*iso*-thiocyanate,
(Allylcarbinyl-*iso*-thiocyanate)
$CH_2=CH—CH_2—CH_2—N=C=S$
(natural material)

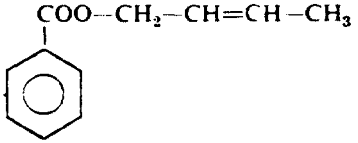
which is a colorless liquid. B.P. 176° C. Sp.Gr. 0.99.

This material is comparatively toxic, irritant and a pronounced lachrymator. Its odor and flavor suggests a use similar to that of common (Allyl-)Mustard oil, and the material finds some use as a modifier of imitation Radish and Garlic flavors.

65-738; 90-843; 140-177;

# 747: CROTYL BENZOATE

Crotonyl benzoate.
*2*-Buten-*1*-yl benzoate.



$C_{11}H_{12}O_2$ = 176.22

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Balsamic-herbaceous, warm odor of moderate tenacity.

This relatively rare ester find some use in perfumery as a modifier in Ambre, Geranium, Fougère and various herbaceous or non-floral fragrance types. Its warm undertones blend very well with Clary Sage, Lavender, Oakmoss, etc. and its balsamic character lends natural nuances to otherwise rough or harsh-chemical odors.

Prod.: from Crotyl chloride plus Sodium benzoate, or:
from Crotyl alcohol with Benzoic acid by azeotropic type esterification.

## 748: CROTYL HEPTOATE

Crotonyl heptylate.
*2*-Buten-*1*-yl heptanoate.

$CH_3(CH_2)_5COO—CH_2—CH=CH—CH_3$

$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

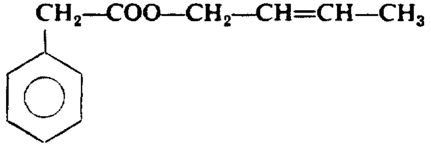
Warm, oily-herbaceous, winey odor of moderate tenacity.

The softness of this odor makes the material immediately attractive, even before one can decide where to use it. And it appears to have the ability to "mellow" and "soften" fragrances with high amount of harsh-smelling chemicals. Its odor type falls within the general picture of Lavender, Chamomile and Clary Sage, but the ester can be used with advantage even in floral types, particularly in conjunction with Ylang-Ylang, Geranium, etc.

Prod.: by direct esterification of *2*-Buten-*1*-ol with Heptanoic acid under azeotropic conditions.

## 749: CROTYL PHENYLACETATE

Crotonyl phenylacetate.
*2*-Buten-*1*-yl-*alpha*-toluate.



$C_6H_5—CH_2—COO—CH_2—CH=CH—CH_3$

$C_{12}H_{14}O_2 = 190.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm and very sweet, Honey-Tobacco-like odor with warm, herbaceous undertones.

This ester, rarely offered commercially, has found a little use in perfume compositions, and it introduces very attractive notes in modern "tabac" fragrance types, particularly with Oakmoss, Vetiver, Lavandin absolute, Clove bud oil, Bergamot, Civet, etc.

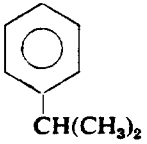
For special effects in certain types of Rose, it supplies absolutely unique undertones, and it can be used at relatively high concentration without causing unpleasant single notes.

The author finds that this ester deserves much more attention and should be tried in perfume compositions by many more perfumers.

Prod.: by direct esterification of *2*-Buten-*1*-ol with Phenylacetic acid under azeotropic conditions.

## 750: CUMENE

*iso*-Propylbenzol.
"Cumol".



$C_6H_5—CH(CH_3)_2$

$C_9H_{12} = 120.20$

Not to be confused with *para*-Cymene (see this).

Colorless mobile liquid. Sp.Gr. 0.86. B.P. 152° C.

Insoluble in water, soluble in alcohol, miscible with oils, almost insoluble in Propylene glycol.

Pungent, slightly green-sharp, kerosene-like odor of poor tenacity.

Occasionally used as a masking agent in industrial perfumes, also as a trace additive in certain artificial essential oils.

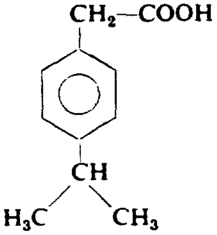
Prod. from Propylene and Benzol in the presence of Aluminium chloride or Boron trifluoride.

Also isolated from Coal tar (petroleum) distillate.

26-662; 68-101; 68-108; 100-298; B-V-393;

## 751: para-CUMENYL ACETIC ACID

"Homo cuminic acid".
*para-iso*-Propyl-*alpha*-toluic acid.
*para-iso*-Propyl phenylacetic acid.



$C_{11}H_{14}O_2 = 178.23$

Colorless or white crystals. Very slightly soluble in water, soluble in alcohol and most oils.

When absolutely pure, the material is virtually odorless, but the scarce commercial lots have shown a distinctly herbaceous odor of considerable tenacity.

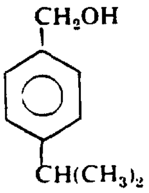
Mildly acidulous and green-herbaceous taste.

The subject material has been mentioned in perfumery literature as suggested for use in perfume compositions. The author is of the opinion that the title material has little or no interest to the perfumer or flavorist. It may be of interest to the perfume chemist if he is involved in the production of related aldehydes of the title material. The material is mentioned here for the sake of contributing (hopefully) to a future elucidation of the nomenclature for the "Cuminic" family. The perfumery literature is particularly confusing on this subject.

Prod.: (several methods) e. g. by oxidation of *para-iso*-Propyl phenylacetaldehyde (a common perfume chemical).

## 752: CUMINALCOHOL

*para-iso*-Propyl benzylalcohol.
Cuminyl alcohol.
Cuminol.
Cumic alcohol.
*para*-Cymen-7-ol.



$C_{10}H_{14}O = 150.22$

Colorless liquid. Very poorly soluble in water, soluble in alcohol and oils. Sp.Gr. 0.98.
B.P. 248° C.

Oily-spicy odor, suggestive of Dillseed or Caraway, but not pungent or sharp like Carvone.

Warm, almost burning, spicy-oily-woody taste.

Occasionally used in perfume compositions for its natural and warm-herbaceous-spicy effect, perceptible in the topnote and often through the dryout. Also used in the artistic duplication of certain floral notes, such as Mimosa and Cassie, particularly in connection with Methylionones.

Finds some use in flavor compositions, mainly Berry, Fruit, Spice and Liquor flavors.

The concentration in the finished product will normally be about 0.5 to 35 ppm.

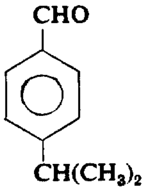
G.R.A.S. F.E.M.A. No.2933.

Prod.: by reduction of Cuminaldehyde, the latter being produced from *para-iso*-Propyl benzoyl chloride plus Hexamethylene tetramine.

26-468; 88-396; 100-299; B-VI-543;
(Also: Givaudan Corp., data sheet).

## 753: CUMINALDEHYDE

*para-iso*-Propyl benzaldehyde.
Cuminal.
Cuminic aldehyde.
Cumaldehyde.



$C_{10}H_{12}O = 148.21$

Colorless liquid. Discolors (yellowish) in presence of iron. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.98 B.P. 236° C.

Pungent, green-herbaceous odor with notes of animal and vegetable character at the same time. Generally described as "unpleasant" in high concentration. At concentrations well below 1% the odor appears more attractive, warm-spicy, still vegetable, condiment-pickle-like.

Although this aldehyde is the chief constituent of Cumin oil, there is a marked difference between the odors of the two materials, the oil having a softness and mellowness in which the high aldehyde content is presented in a very acceptable manner. The Cumin absolute again is strikingly reminiscent of the aroma of the Cumin seed, and will remind many observers of Indian Curry or other spices and condiments. In brief, the Aldehyde represents the sharp nucleus of power and pungency in the Aroma of the oil, the absolute and the seed of Cumin. The aldehyde may therefore appear more "gassy"-kerosene-like to the observer who is familiar with the Aroma of Cumin.

Useful in minute traces in perfume compositions as part of a topnote, however, in most cases, the oil or the absolute are preferred for such delicate creations. On account of its power and very low cost, the Aldehyde also finds use in masking odors for industrial purposes.

More extensively used in flavor compositions as a trace ingredient in Blackcurrant, Gooseberry, Fruit, Spice-blends, etc.

Concentrations is limited to mere traces in the finished product.

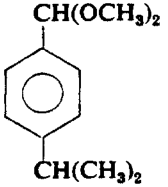
G.R.A.S. F.E.M.A. No.2341.

Prod.: from *para-iso*-Propyl benzoylchloride and Hexamethylene tetramine.

26-662; 77-205; 85-54; 85-126; 89-154; 100-299; 103-254; 103-271; 104-201; B-VII-318; 140-162;

## 754: CUMINALDEHYDE DIMETHYLACETAL

Cuminal-DMA.



$C_{12}H_{18}O_2 = 194.28$

Colorless slightly oily liquid. B.P. 210° C. Sp.Gr. 0.94.

Almost insoluble in water, miscible with alcohol and oils.

Mild, oily-green, herbaceous-winey odor.

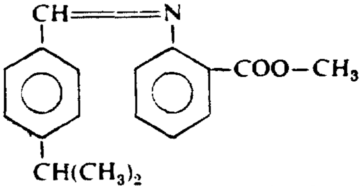
Suggested for use as part of topnote bases in perfume compositions. More stable than the aldehyde, and practically free from the pungent-sharp, hydrocarbon-like notes so dominating in the aldehyde.

Prod.: from Cuminaldehyde plus Methanol with a condensing catalyst.

28-534; 37-282;

## 755: CUMINALDEHYDE-METHYLANTHRANILATE

A "Shiff's Base" type of condensation product.



$C_{18}H_{19}NO_2 = 281.36$

Intensely yellow, somewhat viscous liquid.

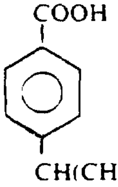
Herbaceous-sweet- very tenacious odor. In dilution reminiscent of Mandarin peel oil, but overall rather sharp and not as "Orangeblossom"-like as most of the conventional Schiff's bases.

The odor is strongly dependent upon the ratio of components used in the condensation, and upon traces of surplus component.

Prod. from Cuminaldehyde and Methylanthranilate by condensation.

## 756: CUMINIC ACID

*para-iso*-Propylbenzoic acid.
Cumic acid.



$C_{10}H_{12}O_2 = 164.21$

White or colorless crystals, melting at 117° C.
Sp.Gr. (liquid) 1.16.

Very slightly soluble in water, somewhat soluble in alcohol, soluble in most oils.

Very faint, green-woody-spicy odor, resembling sap from wood, yet overall dry.

Not very interesting as a perfume material. Its poor solubility, its acidity and not very rare odortype may well rule it out of the "library" for perfumers.

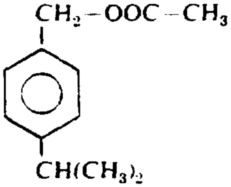
Prod.:

1) by oxidation of Cuminic aldehyde (evt. in presence of water).
2) by oxidation of *para*-Cymene under alkaline or acid conditions.

26-664; 68-545; 100-299; B-IX-546;

## 757: CUMINYL ACETATE

Cuminic acetate.
Cumin acetate.
*para-iso*-Propyl benzylacetate.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Sp.Gr. 1.00. B.P. 251° C.

Very slightly soluble in water, soluble in alcohol and oils.

Refreshing-herbaceous, sweet and delicately woody odor of moderate tenacity.

This ester, much too uncommonly found in the price lists, offers extremely interesting effects for the imaginative perfumer.

Particularly for truly new ideas in perfumery, this ester opens the door to individual creation. Far from being a key material in any existing fragrance, it forms part of many very attractive perfumes.

It blends well with Galbanum, Geranium, Bergamot, Opopanax, Cassie materials, Oakmoss, Ambregris materials, Ionones, etc., and the new esters of the Hexenyl family can add more to some of these combinations.

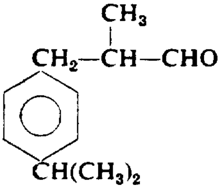
Prod.: by direct esterification of Cumin-alcohol with Acetic acid, or with Acetic anhydride.

90-340;

"Benzylpropylacetate" is G.R.A.S. (162-584), but the confusing name refers actually to Dimethyl carbinyl acetate.

## 758: CYCLAMEN ALDEHYDE

*alpha*-Methyl-*para-iso*-propyl phenylpropionaldehyde.
*2*-Methyl-*3*-(*para-iso*-propylphenyl) propionaldehyde.
*alpha*-Methyl-*para-iso*-propyl hydrocinnamic aldehyde.
Cyclamal.
Cyclosal.
Cyclaviol.
Alpine Violet. (Violet Alpine).
"Lime Aldehyde".
Aldehyde B.



$C_{13}H_{18}O = 190.29$

Colorless oily or slightly viscous liquid. Almost insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol and Glycerin.

Sp.Gr. 0.95. B.P. 270° C.

Diffusive and powerful floral-green floral-stem like odor with pronounced vegetable, Cucumber-Melon-like notes. Overall resembling the odor of Lindenblossom.

Extensively used in perfumery for floral effects, fresh-green-floral topnotes (of lasting fragrance). Useful in Lilac, Lily, Peony, Magnolia, Orangeblossom, Alpine Violet, etc.

Blends well with the Ionones and all Rose notes.

The commercial product is usually stabilized and adjusted to a suitable aldehyde strength, rarely higher than 95%, often about 70%. It is important that the stabilizer does not contribute to the odor of the aldehyde.

Finds some use in flavor compositions, mainly for Citrus and various fruit flavor types. The concentration in the finished product is normally about 0.3 to 1.2 ppm (mere traces).

Prod.: (many methods), e. g.: from Cuminaldehyde plus Propionaldehyde by condensation followed by selective hydrogenation and finally dehydrogenation of the Cyclamen alcohol to aldehyde.

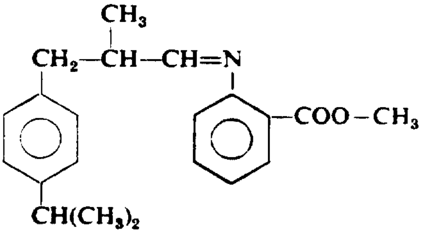
G.R.A.S. F.E.M.A. No.2743.

An interesting analog of Cyclamenaldehyde has been prepared from Anethole.

5-144; 4-37; 86-94; 103-213; 106-126; 156-145; 34-772;

## 759: CYCLAMENALDEHYDE-METHYLANTHRANILATE

"Cyranthiol" (Givaudan).
"Lilianthol".
Methyl-*N*-(*3*-(*para-iso*-propylphenyl)-*2*-methylpropylidene)-anthranilate.
A "Shiff's Base" type of condensation product.



$C_{21}H_{25}NO_2 = 323.44$

Yellowish viscous liquid, barely pourable at room temperature. Almost insoluble in water and Propylene glycol. Soluble in alcohol and perfume oils.

Intensely sweet, fresh-floral odor of great tenacity, somewhat reminiscent of the flowers of the Lemon tree.

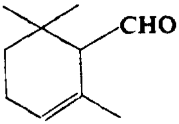
Greener and more diffusive than Hydroxycitronellal-Methylanthranilate.

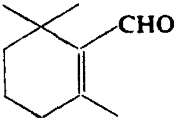
Finds some use in perfume compositions, probably ranking No. 3 among Schiff's bases after Aurantiol and Acaciol. Its fresher odor type and less "Orangeblossom"-character are its main assets.

Prod. by condensation of Cyclamenaldehyde and Methylanthranilate.

## 760: CYCLOCITRAL

*alpha*-Cyclocitral = (*2,2,6*-Trimethyl-*5*-cyclohexen-*1*-carboxaldehyde).
*beta*-Cyclocitral = (*2,2,6*-Trimethyl-*6*-cyclohexen-*1*-carboxaldehyde).
Both isomers are known and have been produced separately.





$C_{10}H_{16}O = 152.24$

*alpha*-
Sp.Gr. 0.92. B.P. 195° C.

*beta*-
Sp.Gr. 0.95. B.P. 200° C.

Colorless liquids.

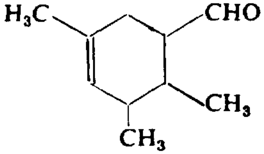
Very rarely offered commercially. These particular Cyclocitrals have little or no interest to the creative perfumer, but they have served as part of many pieces of proof that isomers (*alpha-beta*) do often have different odors.

Prod. by condensation of Citral with Aniline, followed by hydrolysis and separation of the *alpha* and *beta* isomers by fractionated distillation.

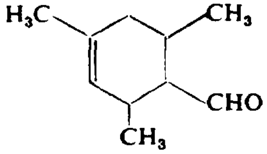
4-38; 5-172; 67-500; 156-105;

## 761: iso-CYCLOCITRAL

A mixture of two chemicals:
*3,5,6*-Trimethyl-*3*-cyclohexen-*1*-carboxaldehyde (*meta*-Cyclocitral).



*2,4,6*-Trimethyl-*4*-cyclohexen-*1*-carboxaldehyde (symmetric-*iso*-Cyclocitral).



$C_{10}H_{16}O = 152.24$

– and isomers of same.
The commercial product is sometimes called: *meta*-Cyclocitral.

Colorless liquid. Insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.93.

Powerful, and diffusive, foliage-green, "dark"-weedy and dry odor, sometimes described as "Flower-shop odor". The earthy and wet-green notes are quite natural in high dilution and resemble the odor of stems from plants and flowers fresh from the soil.

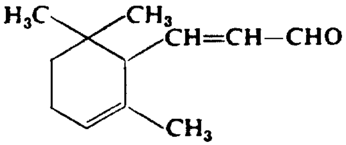
Finds use in perfume compositions where it blends excellently with Oakmoss products (compensates for sweetness and lifts the topnote), with Ionones (freshness), Geranium and Galbanum (enhances the green and "vegetable" notes), etc.

On account of its modest cost it also finds its way into masking odors for industrial purposes. Its power compensates for its cost (usually slightly less than Citral) for such purposes.

Prod. by a Diels-Alder type condensation of *2*-Methyl-*2,4*-pentadiene and Crotonaldehyde. The reaction product is a mixture of isomers commercially called *iso*-Cyclocitral (after rectification).

86-73; 156-372;

## 762: alpha-CYCLOCITRYLIDENE ACETALDEHYDE



$C_{12}H_{18}O = 178.28$

Colorless or pale yellowish oily liquid.

Mild floral-woody, somewhat oily-herbaceous odor, remotely reminiscent of Rose with similarity to the odor of hydrogenated Ionones.

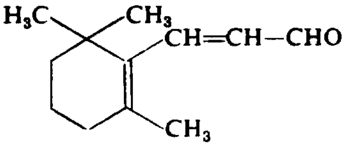
Suggested for use in perfume compositions. It brings a certain amount of floral lift to Rose compositions, and performs fairly well even in soap. However, the cost of the rarely offered and never readily available lots are rather discouraging to the perfumer, and it is most conceivable that this material can be left out of the perfumer's library without any great loss.

Prod. from *alpha*-Cyclocitral and Acetaldehyde by condensation.

5-97;

## 763: beta-CYCLOCITRYLIDENE ACETALDEHYDE

*2,6,6*-Trimethyl-*1*-cyclohexenyl-*beta*-acrolein.



$C_{12}H_{18}O = 178.28$

Colorless or pale yellowish oily liquid.

Sweet-woody, rather heavy odor, resembling that of *beta*-Ionone. More fruity than really floral, but not as tenacious as the Ionone.

Suggested for use in perfume compositions, but since it does not offer any new or unusual odor characteristics, and it cannot be produced in economical competition to *beta*-Ionone, there is little or no chance that it will ever become a standard shelf ingredient for the perfumer.

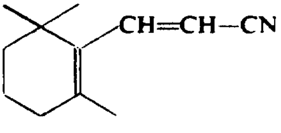
Prod. from *beta*-Cyclocitral and Acetaldehyde by condensation.

5-97;

## 764: CYCLOCITRYLIDENE ACETONITRILE

*beta*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-acrylonitrile.

*beta*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-vinylcyanide.



$C_{12}H_{17}N = 175.28$

Colorless or pale straw-colored liquid.

Insoluble in water, soluble in alcohol and oils.

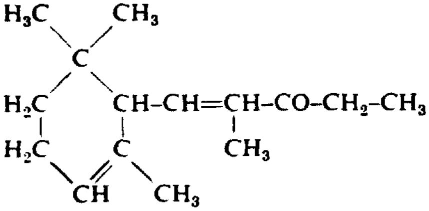
Sweet herbaceous-woody, quite powerful odor with some resemblance to the odor of *beta*-Ionone. More diffusive, less tenacious, and not quite as floral.

This rare chemical has been suggested for use in perfume compositions where Cyclocitrylidene acetaldehyde may have been desirable, but caused trouble in being unstable (alkaline conditions, etc.). However, the need for such odor types is extremely small and very few perfume laboratories seem to carry this material. The title material is fairly stable in alkali, but decomposes under acid conditions.

Prod.: several methods, e. g. from *beta*-Cyclocitral via Grignard synthesis with Cyanogen chloride, or via the aldehyde (see monograph) and its aldoxim by treatment with Thionyl chloride or Acetic anhydride.

## **765:** alpha-**CYCLOCITRYLIDENE**-4-**METHYLBUTAN**-3-**ONE**

*1,3*-Dimethyl-*alpha*-ionone.
*5*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*4*-methyl-*4*-penten-*3*-one.
Dimethyl ionone.
Sometimes called "*iso*-Ethyl-*alpha*-ionone".



$C_{15}H_{24}O = 220.36$

Colorless to pale yellowish oily liquid.
Sp.Gr. 0.92. B.P. 243-249° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

The commercial products are normally mixtures of several isomers. The above structure describes the *alpha*-isomer.

The Dimethylionones have been known and produced since the early days of Ionone research in the beginning of this century. In view of the success of the Methylionones, particularly the *iso*-Methyl-*alpha*-ionone it is understandable that the next higher homologues were under close observation.

Several commercially available specialties consist wholly or mainly of Dimethylionone mixture.

The odor varies according to isomer ratio, but can generally be classified as warm, Violet-like, sweet, yet somewhat powdery and very tenacious.

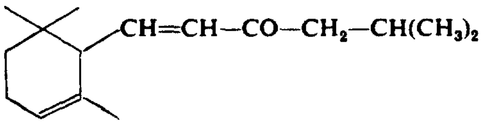
This ketone is used in fine perfumery where warm and powdery, rich, sweet and lasting Ionone-type odors are desirable. This material seems less prone to discoloration or "yellowing" than many of its lower homologues.

Prod.: from Citral and Diethylketone by condensation, followed by cyclization.

86-47; 96-171; 156-203;

## **766:** alpha-**CYCLOCITRYLIDENE**-1-**METHYLPENTAN**-4-**ONE**

*alpha*-Methyl ethyl ionone.
*6*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*1*-methyl-*5*-hexen-*4*-one.
An *iso*-Propylionone.
Commercial products contain various amounts of several isomers. The above name and the structure refer to the *alpha*-isomer.



$C_{16}H_{26}O = 234.38$

Pale yellowish or straw-colored, or almost colorless oily liquid. B.P. 265° C.

Insoluble in water, soluble in alcohol and oils.

The odor of Ionones and their homologues is a subject generally avoided in written publications. Not only is it extremely difficult to give more than a very broad and general odor description without the desirable nuances, but our perfumery language leaves much to be desired with respect to variety in its vocabulary. Variations in odor of materials from different suppliers and even in batches of different age from same supplier further add to the difficulties. The author fully agrees with the late Dr. E. S. Maurer (see 103-267/278) and other authors, that "more than half the Greek alphabet is necessary in order to describe some of the isomers".

Powerful and rich, powdery-velvety odor of considerable tenacity. Overall distinctly different from the odor of *alpha*-Methylionone and other common Methylionones.

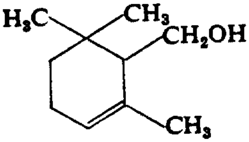
Although this higher homologue is rarely, if ever, offered commercially under its proper chemical name, it has found some use in perfume compositions.

Its unusually clean-powdery, lasting odor can be utilized by careful blending into novel luxury fragrances with macrocyclic musks or Indane-type musks, Ambregris chemicals, Clary Sage derivatives, Oakmoss products, Galbanum, etc. for modern type fragrances.

Prod.: by condensation of Citral with Methyl-*iso*-butylketone, followed by cyclization e. g. with Phosphoric acid.

(See also: 156-203).

## **767:** alpha-**CYCLOGERANIOL**



$C_{10}H_{18}O = 154.25$

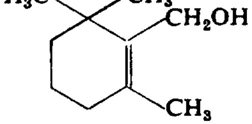
Colorless liquid. B.P. 195° C. Sp.Gr. 0.92.

Soft, floral, sweet odor of rather poor tenacity. In the author's opinion, it is not nearly as useful as Geraniol, although it cannot be compared to Geraniol as any sort of a substitute. It finds use occasionally in perfumes for soaps and detergents, where its lift helps bring the rosy notes out in practical use of the functional product.

Prod.: by cyclization of Geranyl acetate in presence of acid. The reaction product is subsequently hydrolyzed to yield a mixture of *alpha*- and *beta*-Cyclogeraniol. The two isomers are separated by fractionated distillation.

4-38; 5-178; 67-502; 86-37;
(see next monograph).

## **768:** beta-**CYCLOGERANIOL**



$C_{10}H_{18}O = 154.25$

Colorless or pale yellowish, oily liquid.
B.P. 203° C.

Rather minty, fresh and slightly green odor, reminiscent of that of Pulegol, but more Eucalyptus-like, cool, and not very floral. Diffusive and not very tenacious.

Has been suggested for use in perfume compositions, but its overall character does not make it generally attractive, and there are many and less expensive materials that will produce similar notes and effects.

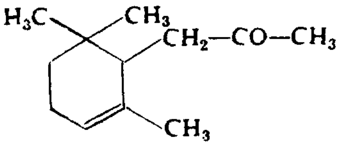
Prod.: from Geraniol via Geranyl acetate, which by acid cyclization gives Cyclogeranyl acetate. The latter is hydrolyzed to yield a mixture of *alpha*- and *beta*-Cyclogeraniol.

4-38; 5-174; 67-502;
(see also previous monograph).

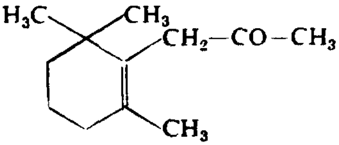
## 769: CYCLOGERANYL METHYLKETONE

(also called: Methyl geranyl ketone).
The *alpha*- and *beta*-isomer have been manufactured separately, but they have quite similar odors:

*alpha:*



*beta:*



$C_{12}H_{20}O = 180.29$

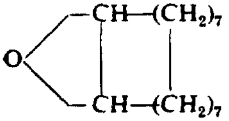
Colorless oily liquids.

Green-camphoraceous odor, both reminiscent of Ionones, but overall sharper, less sweet.

Have been suggested for use in perfume compositions, but are rarely, if ever, offered commercially, and do not seem to have caught the interest of perfumers.

4-38; 103-275; 28-647; 4-90;

## 770: CYCLOHEXADECANE EPOXIDE



$C_{16}H_{30}O = 238.42$

White or colorless crystals. M.P. 61° C.

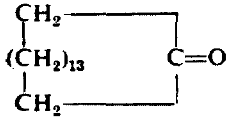
Tenacious, woody-musky, but rather weak odor, not as sweet as Cyclopentadecanone, but more resembling Cyclohexadecanone.

Of little more than acedemic interest. This epoxide does not offer the outstanding qualities of synthetic musk necessary in today's competition with so many excellent musks.

86-37;

## 771: CYCLOHEXADECANONE

"Homoexaltone".



$C_{16}H_{30}O = 238.42$

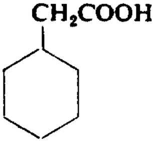
Solid white or colorless mass or white crystals.

Tenacious animal, mostly musk-like odor, more woody and less sweet than Cyclopentadecanone ("Exaltone").

Does not offer sufficiently interesting notes, power or effect that it could compete with the variety of efficient musks available today.

## 772: CYCLOHEXANE ACETIC ACID

Cyclohexyl acetic acid.
Hexahydro phenylacetic acid.



$C_8H_{14}O_2 = 142.20$

Colorless crystalline mass, or white crystals.
M.P. 33° C. B.P. 251° C.

Rather sharp-acetic odor, not very characteristic.

Sour taste, nondescript.

Occasionally used in flavor compositions, mainly for imitation Butter and fruit.

Concentration in the finished product is normally traces.

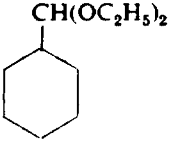
G.R.A.S. F.E.M.A. No.2347.

Prod.: (many methods) e. g. by hydrogenation of Phenylacetic acid.

4-39; 67-224;

## 773: CYCLOHEXANE CARBOXALDEHYDE DIETHYLACETAL

Cyclohexane aldehyde diethylacetal.
Hexahydrobenzaldehyde diethylacetal.
Diethoxy cyclohexylmethane.
Cyclohexylformaldehyde diethylacetal.
Dow Chemical Co., Aromatic No. 58-65.



$C_{11}H_{22}O_2 = 186\ 30$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Earthy-green, sweet, but almost choking, Bitter-almond-like, pungent odor with some resemblance to Nitrobenzene.

Although this acetal can be manufactured at a very low cost, its odor characteristics will place it among the masking odors for industrial purposes. The Dimethyl acetal is more pleasant and generally useful (see next monograph).

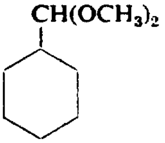
The Cyclohexene carboxaldehyde diethylacetal has been manufactured, and it has an interesting green, Melon-like, wood-sap-like odor. (Dow Chem. Co.).

The title material was made by catalytic hydrogenation of *3*-Cyclohexene aldehyde, followed by Ethanol condensation to make the acetal.

(Dow Chem. Co. 1958).

## 774: CYCLOHEXANE CARBOXALDEHYDE DIMETHYLACETAL

Cyclohexane aldehyde dimethylacetal.
Hexahydrobenzaldehyde dimethylacetal.
Cyclohexylformaldehyde dimethylacetal.
Dimethoxycyclohexyl methane.
Dow Chem. Co. Aromatic No. 58-61.



$C_9H_{18}O_2 = 158.24$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Damp-earthy, camphoraceous-minty, Walnut-Vetiver-Oakmoss-like, relatively powerful odor of moderate tenacity.

This acetal has a more powerful odor than the Diethylacetal (see previous monograph) and it could find use in soap perfumes of the modern woody type, including deodorant soaps, in which the perfume is often of a slightly medicated character, in line with the function of the soap.

Prod.: by condensation of Cyclohexane carboxaldehyde with Methanol e. g. in presence of a small amount of dry hydrogen chloride as water removing agent.

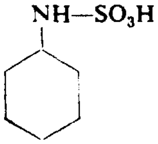
The unsaturated aldehyde, Cyclohexene carboxaldehyde, yields a Dimethylacetal of more earthy, mushroom-like character.

(Dow Chem. Co. 1958).

## 775: CYCLOHEXANE SULFAMIC ACID

"Cyclamic acid".

Cyclohexyl sulfamic acid.



$C_6H_{13}NO_3S = 179.24$

White crystals. M.P. 170° C.

Very poorly soluble in water, decomposes in hot water.

Practically odorless.

Initially sour, then sweet taste (sweet aftertaste).

The sweetness is approximately 30 times that of cane sugar, while the acidity provided by this material is even greater than that derived from an equal weight of Citric acid.

This acid is being used on an increasing scale (1966) as a sweet acidifying agent in soft drinks of no nutritional value (diet-soda, low-calorie carbonated beverages, etc.).

See also Calcium cyclamate and Sodium Cyclamate.

Prod. from Cyclohexylamine by Sulfonation.

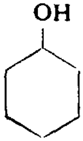
G.R.A.S.

100-310;

## 776: CYCLOHEXANOL

Hexalin.

Hexahydrophenol.



$C_6H_{12}O = 100.16$

Colorless crystal needles, liquefying in moist air, melting at 25° C. B.P. 162° C.

Sp.Gr. 0.96 (liquid).

4% soluble in water, miscible with alcohol and oils. Cyclohexanol will dissolve 11% water at room temperature.

Warm-camphoraceous odor.

Bitter-camphoraceous taste.

Finds some use in masking odors for industrial purposes, but is of little use as such in general perfumery.

Note: Vapours are toxic to human respiratory system, the tolerance being about 100 ppm of Cyclohexanol-vapours in air.

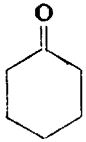
Prod.:

1) by reduction of Cyclohexanone.
2) by hydrogenation of Phenol in the presence of a catalyst. This is the most common commercial method.

26-470; 67-159; 100-310; 1-687; B-VI-5;

## 777: CYCLOHEXANONE

Nadone. (this name also used for 2-Cyclohexyl-cyclohexanone).
Pimelin ketone.
Ketohexamethylene.



$C_6H_{10}O = 98.15$

Colorless oily liquid. B.P. 156° C.
Sp.Gr. 0.95.

Soluble in water, alcohol and oils.

Powerful, minty-camphoraceous, "cool" and "solvent-like" odor, generally described as "unpleasant" (by non-professionals).

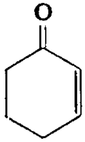
This ketone finds some use in masking odors for industrial perfumery jobs, however, there are times when the problem is that of masking the odor of Cyclohexanone itself in other industrial uses. Extremely stable, except in alcoholic solution, which is easily oxidized to Caproic acid, etc. under influence of daylight.

NOTE: Vapours are irritating to human mucous membranes, and toxic.

Prod.:
1) by partial catalytic hydrogenation of Phenol.
2) by Chromic acid oxidation of Cyclohexanol.

1-694; 26-470; 67-192; 67-196; 100-310; B-VII-8;

## 778: CYCLOHEXEN-2-ONE(1)



$C_6H_8O = 96.13$

Colorless mobile liquid. B.P. 170° C.

Poorly soluble in water, soluble in alcohol and oils.

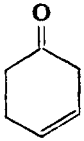
Powerful and diffusive, somewhat gassy-minty odor, often described as "industrial" or "chemical".

Occasionally used as part of masking odors for industrial perfumes.

Prod.: by Chromic acid oxidation of Cyclohexene, this in turn being produced by dehydration of Cyclohexanol.

67-209; 77-211; 86-38;

## 779: 3-CYCLOHEXENONE-1



$C_6H_8O = 96.13$

Colorless mobile liquid.

Slightly soluble in water, soluble in alcohol and oils.

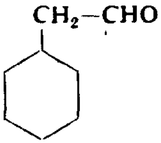
Commercial grades of this ketone have an odor which is most often described as "Urine-like". It is somewhat ethereal, sweet-solvent-like, Acetone-like in purer grade material.

This type of odor is rarely, if ever, called for in perfumery, but the ketone has achieved some academic interest because of its peculiar odor and the fact that it is a natural component of human Urine.

4-39; 67-208; 4-194; 86-144;

## 780: CYCLOHEXYL ACETALDEHYDE

Hexahydrophenylacetaldehyde.



$C_8H_{14}O = 126.20$

Colorless oily liquid. B.P. 163° C.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing green-floral odor of poor tenacity. Mild, yet quite diffusive, overall more sweet-floral than Cyclohexenyl acetaldehyde.

This aldehyde finds some use in perfumery, although only in certain types of fragrances for household products, etc. Its odor type is not suitable for finer perfumes, except as a minor ingredient in aldehydic topnote compositions.

Its power and low cost makes it an attractive item for the volume fragrances intended for detergents, room-sprays, cleaners, etc. It gives pleasant and refreshing effects in Pine needle fragrances, and performs well with all the Citrus oils.

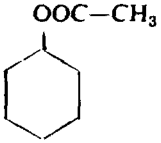
Prod.: (many methods) e. g.

1) from Butadiene by condensation with Crotonaldehyde, followed by hydrogenation.
2) by ozonolysis of *1*-Allylcyclohexan-*1*-ol.
3) from Acetylene via Cyclohexylidene acetaldehyde – by hydrogenation.

67-191; 163-333; (see also: 31-59);

## 781: CYCLOHEXYL ACETATE

"Cyclohexane acetate".
Not to be confused with esters of
Cyclohexane acetic acid.



$C_8H_{14}O_2 = 142.20$

Colorless oily liquid. B.P. 174° C.
Sp.Gr. 0.99.

Insoluble in water, soluble in alcohol and oils.

Sweet-fruity, but rather chemical odor. Often described as similar to Amylacetate, but the odor of Cyclohexyl acetate is sharper, less "candy-like", less "natural".

Sweet-fruity taste, more powerful than that of Amyl acetate.

Rarely used in perfumery, except occasionally in masking odors for industrial purposes.

Finds some use in flavor compositions, mainly for imitation Apple, Blackberry, Banana, Raspberry, and in "Tutti-frutti" flavors.

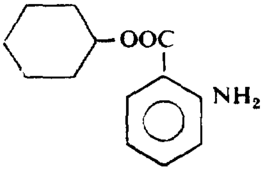
Concentration in baked goods may be as high as 120 ppm, while it is generally lower in carbonated beverages or candy.

G.R.A.S. F.E.M.A. No.2349.

Prod.: from Cyclohexanol by Acetylation.

4-38; 26-470; 86-38; B-VI-7;

## 782: CYCLOHEXYL ANTHRANILATE



$C_{13}H_{17}NO_2 = 219.29$

Pale yellowish liquid. Sp.Gr. 1.01.
B.P. 318° C.

Faint, fruity-Orangeblossom-type odor of good tenacity.

Finds some use in cosmetics as a sunscreening agent. Hardly used in perfumery for its odor.

Sweet-fruity, Grape-like taste.

Used in flavor compositions for imitation Grape, Apple, Banana, etc.

Concentration in the finished product is normally mere traces.

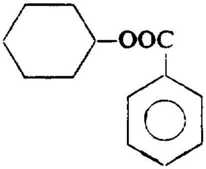
G.R.A.S. F.E.M.A. No.2350.

Prod.: from Isatoic anhydride plus Cyclohexanol.

4-39; 86-38;

## 783: CYCLOHEXYL BENZOATE

Hexahydrophenyl benzoate.



$C_{13}H_{16}O_2 = 204.27$

Viscous liquid. B.P. approximately 282° C.

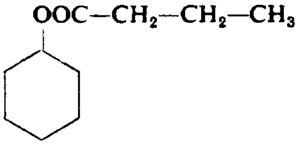
Mild, faint, warm-balsamic, floral and somewhat herbaceous odor of good tenacity. The herbaceous notes appear as undertones barely perceptible except in compositions with other materials.

This ester finds very little use in perfumery.

Prod. directly from Cyclohexanol and Benzoic acid by azeotropic esterification.

86-38; 7-206;

## 784: CYCLOHEXYL BUTYRATE



$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. B.P. 212° C. Sp.Gr. 0.95.

Almost insoluble in water, soluble in alcohol and oils.

Overall fruity, but has a nondescript floral note, remotely reminiscent of Phenoxyethyl isobutyrate. The Cyclohexyl butyrate is, however, much more powerful in its odor, and less tenacious.

Rarely used in perfumery. Could find some use in delicate floral fragrances such as Peony, Sweet Pea, Appleblossom, Magnolia and in powerful bases such as Jasmin.

Used in flavor compositions for imitation Apple, Apricot, Banana, Peach, Strawberry, etc.

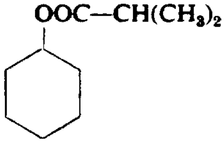
Concentration in the finished product is normally only traces, but may be about 35 ppm in baked goods.

G.R.A.S. F.E.M.A. No.2351.

Prod.: by azeotropic esterification of Cyclohexanol with *n*-Butyric acid.

4-39; 86-38;

## 785: CYCLOHEXYL-iso-BUTYRATE



$C_{10}H_{18}O_2 = 170.25$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity odor, more ethereal-diffusive than Amyl acetate, sweeter, but overall resembling that ester in odor. The background appears almost Oriental-animal or Ambra-like.

Finds some use in perfumery, mainly in Chypre, Ambre, Oriental compositions, and it blends well with Patchouli, Myrrh, Opopanax, Labdanum, Jasmin, etc.

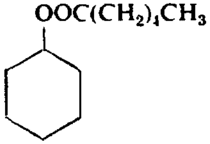
Intensely sweet taste, more powerful than that of Amylacetate and richer than Amylbutyrate. It blends well with Amyl acetate and -butyrate.

Finds some use in flavor compositions, mainly for imitation Apple, Pineapple, Peach, etc., and in "Juicy-fruit" and similar complexes.

Prod. by direct esterification of Cyclohexanol with *iso*-Butyric acid.

4-39; 77-186; 140-139;

## 786: CYCLOHEXYL CAPROATE



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Fruity-winey, but somewhat "metallic" odor of considerable tenacity. Overall resemblance to Pineapple-fruity odors.

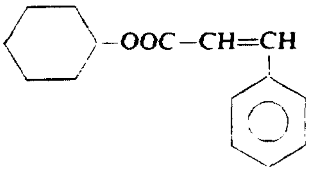
Finds some use in perfume compositions as part of a fruity topnote in modern mossy-aldehydic fragrance types.

Used in flavor compositions for imitation Apple, Pineapple, Brandy, Cognac, Arak, etc.

Prod.: by direct esterification of Cyclohexanol with Caproic acid.

86-38;

## 787: CYCLOHEXYL CINNAMATE



$C_{15}H_{18}O_2 = 230.31$

Colorless viscous liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol, miscible with most perfume and flavor materials.

Sweet-balsamic, somewhat Almond-like and very tenacious odor. The "Almond-like" note resembles that of Heliotropyl esters with a touch of Benzaldehyde-note. The balsamic note resembles that of Benzyl cinnamate.

Finds very little – if any – use in perfume compositions.

Occasionally used in flavor compositions, mainly for imitation Cherry, Peach, Prune, Apricot and Apple.

Concentration in baked goods may be as high as 20 ppm, but is generally lower in other consumer products.

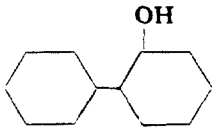
G.R.A.S. F.E.M.A. No.2352.

Prod.: by azeotropic esterification of Cyclohexanol with Cinnamic acid.

4-39; 77-195;

## 788: 2-CYCLOHEXYL CYCLOHEXANOL

Exists in *cis*- and *trans*-form.
Both are available in high purity.
The *cis*-form is commercially preferred.



$C_{12}H_{22}O = 182.31$

Colorless oily liquid.

Woody-camphoraceous, slightly minty and rosy odor, but overall dry and rather "chemical".

Slightly bitter taste.

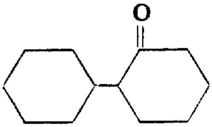
Little, if any, interest for perfumers. However, this alcohol is occasionally used in cosmetic formulations as a mild insect repellant to compensate for the insect attractant effect of certain sunscreening agents.

Prod.: by hydrogenation of 2-Cyclohexyl cyclohexanone (see next).

Litt.: Allied Chemical Co. (U.S.A.) data sheet No. D. 21, 1962.

## 789: 2-CYCLOHEXYL CYCLOHEXANONE

*ortho*-Bicyclohexanone.
"Lavamenthe" (Dow Chem. Co.).
"Givmenthe" (Givaudan Corp.).
"Nadone" (Allied Chemical Co.) – this name was earlier used for Cyclohexanone.



$C_{12}H_{20}O = 180.29$

Colorless liquid. B.P. 264° C.
Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Herbaceous-minty, comparatively sweet odor, overall pleasant and of great tenacity.

Minty, somewhat dry taste. Slightly bitter in higher concentrations but bitterness is less pronounced in compositions with other flavoring materials or at lower concentration.

Has found some use in perfume compositions, partly due to its excellent stability in soap and good stability towards other chemically active functional products. For Lavender, Rose, Chypre and Fougères in particular, and in general to introduce power and "lift" to soap of detergent perfumes.

Taste: Minimum perceptible: about 3 ppm in 10% sugarwater.

Suggested use level, when used in compositions: 30 to 100 ppm. Effective level – but no cooling sensation: 10 to 30 ppm.

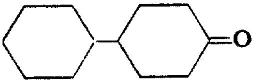
NOTE: It is important that this ketone is fairly free from the *para*-isomer (see next) particularly if it is to be used in flavors.

This ketone has found quite extensive use in dentifrice flavor compositions, where it can support the Mint notes and introduce unusual power at concentrations up to 1100 ppm in the dentifrice.

Litt.: Allied Chemical Co. – data sheet No. D. 21, 1962.

## 790: 4-CYCLOHEXYL CYCLOHEXANONE

*para*-Cyclohexyl cyclohexanone.
*para*-Bicyclohexanone.
"Product C-66" (Dow Chem. Co.).



$C_{12}H_{20}O = 180.29$

Colorless, slightly oily liquid.

Woody-camphoraceous, faintly herbaceous, but rather dry odor.

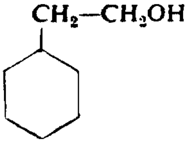
Camphoraceous, bitter-dry taste.

This ketone finds little or no use as such in perfumes or flavors, but it is important to know its odor and flavor in order to properly evaluate the quality of the *ortho*-isomer (see previous monograph).

The *para*-isomer is a common impurity in the crude reaction product, Cyclohexyl cyclohexanone, and should be quantitatively separated from the *ortho*-isomer, if possible.

## 791: CYCLOHEXYL ETHYLALCOHOL

2-Cyclohexyl ethanol.
Hexahydro phenylethylalcohol.



$C_8H_{15}O = 127.21$

Colorless oily liquid. B.P. 204° C.

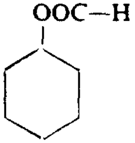
Dry-camphoraceous odor with some (but not much) resemblance to Rose and Patchouli notes.

Suggested for use in soap perfume compositions. It is very stable and does not produce the "gassy" deterioration notes often encountered in Phenylethyl alcohol. However, being a product based upon Phenylethyl alcohol, it comes at a higher price and its odor type does not justify this. Its complete lack of floral sweetness has limited its use considerably.

Prod.: By catalytic hydrogenation of Phenylethylalcohol under pressure.

67-179;

## 792: CYCLOHEXYL FORMATE



$C_7H_{12}O_2 = 128.17$

Colorless liquid. Sp.Gr. 1.00.

Very slightly soluble in water, miscible with alcohol and oils. Sweet-fruity, fruit-preserver-like odor.

Sweet, "jam-like" taste.

The author is not aware of its use in perfume compositions.

This ester has found some use in flavor compositions, mainly in imitation Cherry and Plum.

Concentration in the finished product is normally only traces.

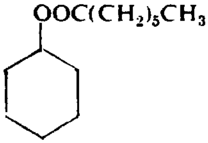
G.R.A.S. F.E.M.A. No.2353.

Prod.: by direct formylation of Cyclohexanol.

4-39; 5-247; 86-38;

## 793: CYCLOHEXYL HEPTOATE

Cyclohexyl heptylate.
Cyclohexyl oenanthate. (This name also refers to the ester with mixed fatty acids).



$C_{13}H_{24}O_2 = 212.34$

Colorless liquid. B.P. 265° C. Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils.

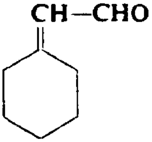
Oily-herbaceous, grassy and slightly fatty, overall not very pleasant odor.

Has found some use in perfume compositions, mainly as part of Citrus topnote compositions or bases for Lemon and Bergamot.

Prod.: By azeotropic esterification of Cyclohexanol with Heptanoic acid.

4-39; 86-38;

## 794: CYCLOHEXYLIDENE ACETALDEHYDE



$C_8H_{12}O = 124.18$

Colorless liquid. B.P. 187° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, refreshing, sweet-floral odor of poor tenacity. It has been classified as "nondescript" and it is true that the material has an odor which is difficult to describe, but it should not be understood as "bland" or "mild".

This aldehyde has been suggested for use in perfume compositions, but its high volatility makes it problematic except for usage in certain types of industrial masking odors, and the aldehyde is too expensive for such low-cost formulations.

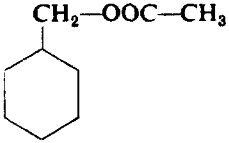
As a trace component in Citrus compositions, or in citrusy topnote bases, it may give quite interesting effects, and it is quite possible that it forms part of certain specialties of that type.

Prod.: (many methods) e. g. by ozonolysis of *1*-Allylcyclohexan-*1*-ol. (a certain amount of Cyclohexyl acetaldehyde is also formed). Other methods are based upon Acetylene synthesis.

31-59; 67-191;

## 795: CYCLOHEXYL METHYLACETATE

Hexahydro benzylacetate.
"Cyclohexane methylacetate".



$C_9H_{16}O_2 = 156.23$

Colorless mobile liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Pronounced fruity and somewhat floral (Jasmin) odor. Overall sweeter and more tenacious than Benzyl acetate.

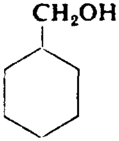
Finds some use in perfume compositions. partly for its fruity notes in lipstick compositions and in masking odors, partly for its Jasmin-like notes in low-cost floral fragrances for detergents, etc. It can partly or wholly replace Benzyl acetate in variations of Gardenia.

Not approved for food use in the U.S.A.

Prod.: By azeotropic esterification of Cyclohexyl Methylalcohol with Acetic acid.

## 796: CYCLOHEXYL METHYLALCOHOL

NOTE: Not to be confused with Methyl cyclohexanol.
Cyclohexyl methanol.
Cyclohexyl carbinol.
Hexahydro benzylalcohol.



$C_7H_{14}O = 114.19$

Colorless oily liquid. B.P. 181° C.

Very slightly soluble in water, soluble in alcohol and oils.

Musty-champhoraceous, slightly minty odor, remotely reminiscent of part of the Patchouli odor-picture.

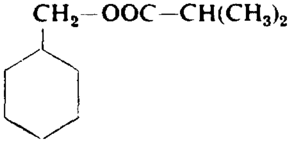
Has found some use in soap perfume compositions, partly due to its good stability. It introduces good power and diffusion in Pine, Wood and Leather notes, and blends well with Cedarwood, Ionones, Rose chemicals, etc.

Prod.: by catalytic hydrogenation of Methylbenzyl ether.

67-178;

## 797: CYCLOHEXYL METHYL-iso-BUTYRATE

Hexahydrobenzyl-*iso*-butyrate.



$C_{11}H_{20}O_2 = 184.28$

Colorless, slightly oily liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Delicately fruity, Pineapple-Apricot-like odor of good tenacity. Tealike, almost Clary Sage-like undertones.

The taste is generally fruity, but not very sweet, yet practically free from camphoraceous or woody notes.

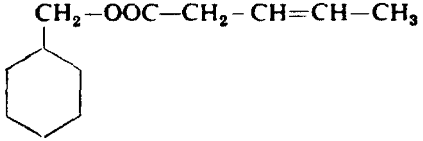
The above ester has been suggested for use in perfume compositions as a modifier for fruity notes, to increase the tenacity of same, and to introduce a different type of sweetness. It blends very well with the Ionones and it supports Benzyl acetate in Jasmin types, introduces freshness in lipstick perfumes, etc.

Not yet approved for food use in the U.S.A.

Prod.: by direct esterification of Cyclohexyl methanol with *iso*-Butyric acid.

## 798: CYCLOHEXYL METHYLCROTONATE

Hexahydrobenzyl-*trans-2*-butenoate.
Hexahydrobenzyl-*beta*-methylacrylate.
Cyclohexylmethanol, *alpha*-crotonic ester.



$C_{12}H_{20}O_2 = 196.29$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Fruity, slightly oily, bitter-sharp, rather pungent odor with a pleasant herbaceous-winey undertone.

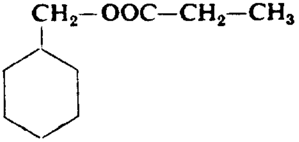
Has been suggested for artificial Chamomile, etc. in perfume bases.

Commercial samples have, however, so far shown too much of "acrylic" off-odors, and it is unlikely that the material will gain any popularity unless it is offered in high purity and stable form.

Info.: DOW Chem. Co., Aromatics, 1957.

## 799: CYCLOHEXYL METHYLPROPIONATE

Hexahydrobenzyl propionate.



$C_{10}H_{18}O_2 = 170.25$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Fruity-herbaceous, berry-like, slightly camphoraceous odor reminiscent of notes in Geranium and Lavender.

Dry-fruity, somewhat camphoraceous, not very pleasant taste, yet very powerful, and in concentrations below 2 ppm it shows pleasant Banana-Raspberry-notes.

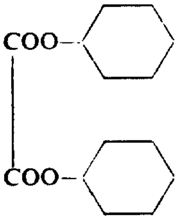
Interesting and powerful material for herbaceous and floral-herbaceous or floral-fruity fragrance types. In general, it will introduce power and lift to such fragrances, and it performs well in fresh detergent perfumes, etc.

Not yet approved for food use in the U.S.A.

Prod.: by direct esterification of Cyclohexyl methanol with Propionic acid.

## 800: CYCLOHEXYL OXALATE

Dicyclohexyl oxalate.



$C_{14}H_{22}O_4 = 254.33$

White crystals or colorless crystalline mass. M.P. 35° C. B.P. 308° C.

Poorly soluble in water, soluble in alcohol and oils.

Almost odorless as such, but introduces a mild-herbaceous odor in compositions. It has, for example, a good influence upon Terpineol and Amyl salicylate in low-cost Fougeres, where it may round off the roughness of the two chemicals and produce a mellower, softer, but not less powerful composition.

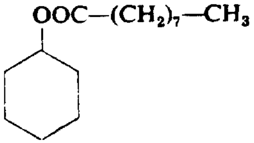
Rarely used in perfumery.

Prod.: by direct esterification of Cyclohexanol with Oxalic acid.

4-39;

## 801: CYCLOHEXYL PELARGONATE

Cyclohexyl nonanoate.
Cyclohexyl nonylate.



$C_{15}H_{28}O_2 = 240.39$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. B.P. 285° C.

Faint, but tenacious, oily-fruity odor with a green-winey undertone.

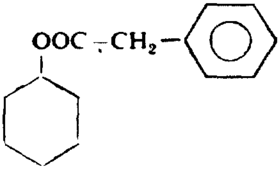
Could find some use in Citrus compositions, Chypres, aldehydic-modern blends, etc.

Rarely used in perfumery.

Prod.: by direct esterification of Cyclohexanol with Nonanoic acid.

4-39;

## 802: CYCLOHEXYL PHENYLACETATE



$C_{14}H_{18}O_2 = 218.30$

Colorless liquid, almost insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.04. B.P. 290° C.

Herbaceous-green, very tenacious odor with sweet-honey-waxy and somewhat Chrysanthemum-like notes.

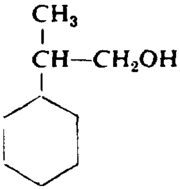
Sometimes used as a fixative for Rose, Chypre, Oriental fragrances etc.

Prod.: by azeotropic esterification of Cyclohexanol with Phenylacetic acid and a catalyst.

4-39; 5-271; 86-38;

## 803: 2-CYCLOHEXYL PROPANOL

Hexahydro hydratropic alcohol.
*2*-Methyl-*2*-cyclohexylpropan-*1*-ol.



$C_9H_{18}O = 142.24$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Very mild-balsamic, floral odor of moderate to poor tenacity.

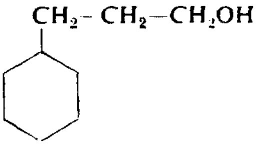
Hydrogenation of known and successful perfume chemicals is one of the many routines of perfume chemical research. Hydrogenation of unpleasant-smelling, inexpensive industrial chemicals is another. In some cases, the result can be precalculated with fair accuracy. In the above case, one would expect to obtain a material inferior to Hydratropic alcohol, which is already a relatively mild odorant of limited application in perfumery.

It is probably reasonable to claim that the title material has failed to interest the perfumers, and it is practically obsolete today.

Prod.: by catalytic hydrogenation of Hydratropic alcohol.

## 804: 3-CYCLOHEXYL PROPANOL

Hexahydro phenylpropylalcohol.



$C_9H_{18}O = 142.24$

Colorless oily liquid.

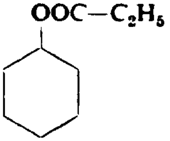
Almost insoluble in water, soluble in alcohol and oils.

Very mild, sweet-balsamic, but rather "flat" odor of moderate to poor tenacity. It is less floral than Hydrocinnamic alcohol, and does not have the rosy character of that material.

The comments made under monograph 2-Cyclohexyl propanol could be repeated in this place. The title material has not been able to catch the interest of the perfumers, and it is generally considered too weak and too expensive for its yield of odor and overall type.

Prod.: by catalytic hydrogenation of Hydrocinnamic alcohol. It can also be prepared directly from Cinnamic alcohol by complete hydrogenation.

## 805: CYCLOHEXYL PROPIONATE



$C_9H_{16}O_2 = 156.23$

Colorless slightly oily liquid. B.P. 195° C.

Almost insoluble in water, soluble in alcohol and oils.

Intensely fruity and sweet odor, somewhat reminiscent of Banana, Pineapple and Peach. Not very tenacious.

Rarely, if ever, used in perfumery.

Occasionally used (in mere traces) in flavor compositions, mainly for Pineapple imitation and similar fruit flavors.

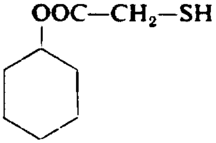
G.R.A.S. F.E.M.A. No.2354.

Prod.: directly by azeotropic esterification of Cyclohexanol with Propionic acid.

4-39;

## 806: CYCLOHEXYL THIOGLYCOLATE

Cyclohexyl mercaptoacetate.



$C_8H_{14}O_2S = 174.27$

Colorless, somewhat viscous liquid.

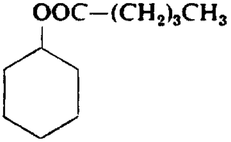
Mild and agreeable, slightly fruity and sweet odor.

Overall weak and rather uninteresting. Of little more than academic interest.

Prod.: by azeotropic esterification of Cyclohexanol with Thioglycollic acid.

34-1245;

## 807: CYCLOHEXYL VALERATE



$C_{11}H_{20}O_2 = 184.28$

Colorless, slightly oily liquid. Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Fruity, slightly animal, deep-herbaceous odor.

Fruity, berry-like taste.

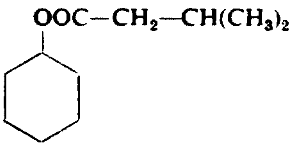
Finds some use in perfume compositions in floral-fruity fragrance types. Blends well with Ionones, Cyclamal, Geranyl esters, etc. and has a fair tenacity. Comparatively stable in soap.

Could find use in flavor compositions for certain type of imitation berry, such as Blackcurrant, which is very difficult to reproduce artificially.

Prod. by direct esterification of Cyclohexanol with *n*-Valeric acid.

4-39; 5-238;

## 808: CYCLOHEXYL-iso-VALERATE



$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol. Sp.Gr. 0.93.

Fruity odor, but less animal than that of the *n*-Valerate. Tenacious and sweet, more versatile than the *n*-Valerate.

Finds little or perhaps no use in perfumery.

Used in flavor compositions for imitation Apple, Strawberry, Raspberry, etc.

Concentration in the finished product (e. g. baked goods) may be as high as 60-70 ppm.

G.R.A.S. F.E.M.A. No.2355.

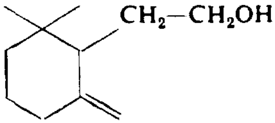
Prod. by direct esterification of Cyclohexanol with *iso*-Valeric acid.

4-39; 5-238;

## 809: gamma-CYCLO HOMOGERANIOL

*1,1*-Dimethyl-*2* (*beta*-hydroxyethyl)-*3*-methylenecyclohexane.

*2*-(*6,6*-Dimethyl-*2*-methylene)-cyclohexylethanol.



$C_{11}H_{20}O = 168.28$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, sweet-Ambregis type odor of moderate to good tenacity.

This material supplies part of the very desirable "maritime" odor of Ambregris. The "seashore" type odor has often been a challenge to the perfumer who wanted to introduce a "novel" note instead of Oakmoss etc. Nerol has been used to imitate the seashore type odor, but it only gives a very modest part of that olfactory picture.

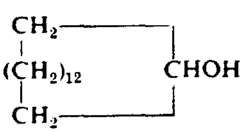
The title material has been manufactured by synthetic way, but it is not yet offered commercially under its proper chemical name. It is used in bases and specialties of Ambregris type odor.

163-323;

See monograph: Ambrinol (footnote) for references to materials of related odor and structure.

## 810: CYCLOPENTADECANOL

Nor-muscol



$C_{15}H_{30}O = 226.41$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Weak, musky odor.

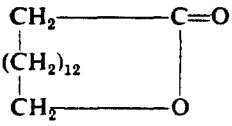
This material has only little more than academic interest, since it has been identified as a component of the Musk from Louisiana (American) muskrats. This Musk was suggested as a substitute for Tibet Muskdeer Musk during World War II in the U.S.A., but the Muskrat Musk was found to be much weaker than the Himalayan Musk.

The oxidation product (by Chromic acid oxidation) is a known commercial Musk chemical, "Exaltone" or "Muscosyn" (Normuscone).

5-201; 156-254; 156-259;

## 811: CYCLOPENTADECANOLIDE

*omega*-Pentadecalactone.
"Angelica Lactone" (misleading name).
Fortolide (Norda).
Exaltolide (Firmenich).
Thibetolide (Givaudan).
Muscolide (Dr. Vogt).
Muscolacton (I.F.F.-Holland).
Pentadecanolide.
*15*-Hydroxypentadecanoic acid, Lactone.
*14*-Oxy-tetradecane carbonic acid, Lactone.
"Pentalide" (Soda Aromatic Co., Ltd., Japan).



$C_{15}H_{28}O_2 = 240.39$

Solid, colorless, crystalline mass, melting at 36-37° C. to a colorless, viscous oil.
B.P. 280° C.

Delicately animal, musky and sweet, extremely tenacious odor of outstanding uniformity. Its fixative effect is absolutely unusual in that it is not a physical fixation, but a true fixative and mellowing effect at incredibly low concentration of usage. The effect of perfumes containing this Lactone differ from others in the excellent "wearability" introduced by the Lactone. This is particularly conspicuous when the perfume is applied to the skin.

Common use level in the perfume oil is about 0.1 to 0.4%.

Cyclopentadecanolide gives highly interesting effects when applied to certain flavors, e. g. alcoholic beverages, dentifrice flavors etc. There is very often a unanimous preference for the flavor that is properly treated with the Lactone.

Concentration in such flavors may be about 0.02 to 1.50 ppm calculated upon the finished consumer product. However, it should be kept in mind, that dentifrices are flavored at extremely high concentration (about 1 %) and it may therefore give an underestimated evaluation of the power of this Lactone. The most frequent abuse of Cyclopentadecanolide is that of over-dosage.

Also used extensively in Berry flavors, Liquor, Wine, Brandy, Fruit, Nut, Vanilla compositions, etc.

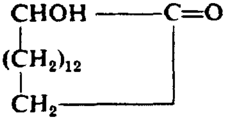
Prod.:
1) by oxidation of Cyclopentadecanone.
2) from linear polyesters of Pentadecanoic acid.

G.R.A.S. F.E.M.A. No.2840.

1-268; 4-50; 5-201; 7-177; 30-275; 31-178; 31-296; 86-39; 90-668; 100-442; 103-195; 106-337; 156-250; 156-259; 140-155; Firmenich data sheet.

## 812: CYCLOPENTADECANOLONE

Hydroxy pentadecanone.



$C_{15}H_{28}O_2 = 240.39$

Colorless crystalline mass or white crystals.

Sp.Gr. 0.96 (liquid). M.P. 58° C.
B.P. 327° C.

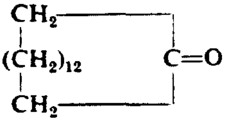
Musky, somewhat animal odor, much weaker than that of Cyclopentadecanolide.

This macrocyclic musk has only little more than academic interest, since it does not display the power of related and equally expensive materials.

4-39; 67-276; 86-39;

## 813: CYCLOPENTADECANONE

"Exaltone" (Firmenich & Cie.).
Muscosyn.
Nor-muscone.



$C_{15}H_{28}O = 224.39$

Colorless or white crystal needles.
M.P. 63° C. B.P. 306° C. Sp.Gr. 0.92.

Practically insoluble in water, soluble in alcohol and oils.

Powerful musky odor, very similar to that of Muscone (Methylcyclopentadecanone) and, in the opinion of many perfumers, superior in type and beauty.

It ranks among the finest and most efficient fixatives known, and – like Cyclopentadecanolide – it improves the "wearability" of a perfume when properly incorporated in the fragrance. Its power becomes more perceptible and evident in extreme dilution, e. g. below one percent in the perfume oil.

Without being a flavor material, – it actually has a rather perfumey and undesirable taste – it has the ability of improving the acceptability of flavors to a remarkable degree. If the flavor is already agreeable and acceptable, the correct amount of Cyclopentadecanone added can eventually bring this "bouquetted" flavor further up and above any similar flavor that does not have the additive.

The concentration of Cyclopentadecanone in alcoholic beverages as a flavor improver may be as low as 0.03 ppm. A somewhat higher level is needed in dentifrice or candy, chewing gum, etc.

Prod.:

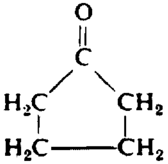
1) by pyrolysis of rare metal salts of dicarboxylic acids.
2) by cyclization (condensation) of dicarboxylic acids in high dilution, using di-Nitriles before cyclization, then hydrolysis.
3) by intramolecular condensation of Bromo acylacetic ester of a dicarboxylic acid. The cyclic ester formed is then hydrolyzed and finally decarboxylated.

– and other methods: (oxidation of Normuscol from Muskrat).

1-755; 4-39; 5-201; 67-270; 156-250;

## 814: CYCLOPENTANONE

Ketocyclopentane.
Adipic ketone.
Keto-pentamethylene.
Dumasin.



$C_5H_8O = 84.12$

Colorless oily liquid. Soluble in water, miscible with alcohol and oils. Very unstable in acid media, polymerizes easily in air.
Sp.Gr. 0.95. B.P. 131° C.

Diffusive, gassy, woody, musty odor. Generally described as unpleasant "industrial".

Rarely used as such, except occasionally as part of masking odors for industrial purposes.

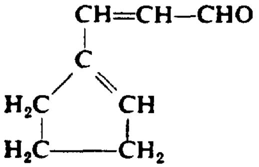
The vapours are considered somewhat toxic.

Prod.: by dry distillation of Adipic acid in presence of metal catalyst.

4-39; 26-470; 67-92; 100-313; B-VII-5;

## 815: CYCLOPENTENYL ACROLEIN

*3*-(Cyclopenten-*1'*-yl)-propen-*2*-al-*1*.



$C_8H_{10}O = 122.17$

Colorless mobile liquid. Almost insoluble in water, soluble in alcohol and oils.

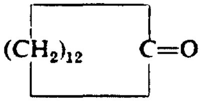
Powerful, sweet-herbaceous, diffusive odor of relatively poor tenacity. In high concentration rather gassy and not very pleasant, it develops sweet and agreeable notes upon dilution.

The material has been suggested for use in perfume compositions, but it is rarely available from the regular suppliers of perfume and flavor chemicals.

In view of its poor keeping qualities, there is not much chance that this material will become a common or desirable item for the perfumer.

Prod.: by condensation of Acetaldehyde with Cyclopent-*1*-ene-*1*-aldehyde. The latter aldehyde can be prepared by a number of methods, e. g. by pyrolysis of Divinyl glycol.

## 816: CYCLOTRIDECANONE



$C_{13}H_{24}O = 196.34$

Colorless oily liquid or colorless crystalline mass. M.P. 32° C. B.P. 250° C.

Insoluble in water, soluble in alcohol and oils.

Woody, rather dry odor. Only in extreme dilution will a musky odor appear clearly.

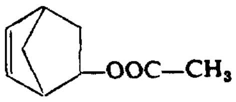
This ketone has mainly academic interest in the study of relationship between chemical structure and musk odor. It is rarely, if ever, used in perfume compositions. Its inferior strength and lack of sweet-animal notes rules it out of the necessary library for the creative perfumer.

Prod.: analogous to Cyclopentadecanone (see this).

30-272; 31-104; 67-270;

## 817: CYCLYL ACETATE

Norbornylenyl acetate.
Bicycloheptenyl acetate.
Norcamphenyl acetate.



$C_9H_{12}O_2 = 152.20$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Pleasant, mild-piney, camphoraceous-woody odor of moderate to poor tenacity.

This ester, developed from very inexpensive, commercially available materials, has found increasing use in perfume compositions, mainly in the "volume products", fragrances for every-day household products, detergents, soaps, etc.

It offers an attractive variation from *iso*-Bornylacetate, and is definitely free from the "Celluloid"-type odor often found in lower grade, low-cost *iso*-Bornylacetates.

The title ester blends very well with all the Pine needle oils, Cyclohexanol derivatives, Sandalwood chemicals, etc. for refreshing or sweet woody odors.

A milder version is Dihydrocyclyl acetate and its corresponding alcohol (see those monographs).

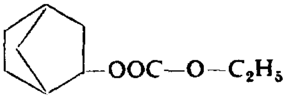
The ester is related to Santenyl acetate which has attracted quite some interest within the past few years.

Prod.: by condensation of Cyclopentadiene with Vinylacetate.

67-340;

## 818: CYCLYL ETHYLCARBONATE

Norbornylenyl ethylcarbonate.
Bicycloheptenyl ethylcarbonate.
Norcamphenyl ethylcarbonate.



$C_{10}H_{14}O_3 = 182.22$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

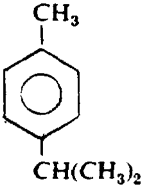
Mild, ethereal-piney, sweet-camphoraceous odor of moderate to poor tenacity.

This ester finds use in perfumery as a fresher, more radiant version of the acetate (see previous monograph). The ethereal character of its odor makes it applicable in herbaceous fragrance types, Lavender, Rosemary, Lavandin, besides of the woody and piney types. It helps soap perfumes perform with more lift and diffusive power, and its low cost makes it attractive to the soap perfumer.

Prod.: from Ethyl chloro formate plus Ethylalcohol plus Norcamphenol. The latter will usually have to be produced by saponification of its acetate (see previous monograph).

## 819: para-CYMENE

Cymene.
Cymol (confusing name occasionally used).
*para*-Methyl-*iso*-propylbenzene.
*para*-*iso*-Propyltoluene.



$C_{10}H_{14} = 134.22$

Colorless mobile liquid. Insoluble in water, soluble in alcohol, miscible with oils.
Sp.Gr. 0.86. B.P. 179° C.

Commercial grades display a typical "gassy"-kerosene-like odor, while highly purified material smells more citrusy, reminiscent of Lemon and Bergamot topnotes, having more freshness.

Commercial grades find extensive use as masking agent in odors for industrial masking purposes, while the pure grade is used in imitation Lemon and Bergamot for perfumes and flavors. It finds some use in low-cost soap and detergent perfumes.

Traces are used in Citrus and Spice flavor blends, while the concentration of *para*-Cymene in chewing gum may reach 250 ppm and in condiments about 125 ppm (pickles etc.).

Prod.:

1) as a by-product in Sulfate-terpentine from paper pulp manufacturing from Spruce wood (U.S.A., U.S.S.R., Canada, Finland, etc.).
2) by dehydrogenation of *d*-Limonene with a catalyst.
3) by catalytic disproportionation of Dipentene.

G.R.A.S. F.E.M.A. No.2356.

26-470; 34-806; 68-101; 68-109; 100-315; B-V-420;
Data sheets and information from:
The Glidden Co.
Hercules Powder Co.
Newport Div.

## 820: DECA-2,4-DIENAL

Heptenyl acrolein.

$CH_3(CH_2)_4CH{=}CH{-}CH{=}CH{-}CHO$

$C_{10}H_{16}O = 152.24$

Colorless, oily liquid.

Almost insoluble in water, soluble in alcohol, poorly soluble in Propylene glycol, miscible with oils.

Extremely powerful, Orange-like, sweet and fresh-citrusy odor, diffusive, yet quite tenacious. The Orange character is more attractive and natural at dilutions below 0.1%, while higher concentrations display fatty-green notes.

Grapefruit-Orange-like taste in extreme dilution in acidified sugarwater.

Identified as a volatile flavor component of fried potatoes.

A comparatively new and very interesting chemical, useful in perfume compositions to beautify a Citrus topnote, to emphasize Bitter Orange character, etc.

Useful in flavor compositions for Grapefruit imitations, etc.

NOTE: Not yet approved in the U.S.A. for food use (1967).

Prod.: by condensation of Hexaldehyde with Croton aldehyde.

89-49; 157-372; 157-378;
Data and information from Compagnie Parento, N. Y. (U.S.A.).

## 821: 2,4-DECADIENOIC ACID

$CH_3(CH_2)_4CH{=}CH{-}CH{=}CH{-}COOH$

$C_{10}H_{16}O_2 = 168.22$

Colorless liquid, insoluble in water, soluble in alcohol and oils.

Fatty, but sweet and very tenacious odor with a pleasant fruity freshness in extreme dilution. In fact, this acid can only be evaluated in dilutions of about 0.1% or lower for odor, and 0.001% (10 ppm) or lower for flavor.

The taste in concentrations of about 5 ppm is fruity, refreshing and slightly oily.

This acid, which has been identified in many natural products, free and esterified, has been made available as a flavor (or perfume) chemical. It is suggested for use in flavor compositions, and its unusual versatility places it as a trace ingredient in a multitude of flavor types: Pear, Peach, Cream, Butter, Milk, Coconut, Chocolate and many other types, including Peanut and Cheese.

The subject acid has not yet (1968) been officially approved for food flavor use in the U.S.A.

Prod.: (several methods) e. g. from *alpha-beta*-Octenal by Reformatzky reaction. Other methods are based upon the Malonic acid – Crotonaldehyde synthesis used in making Hexadienoic acid (Sorbic acid).

158-95;
See also: *2,4*-Decadienal.

## 822: DECADIENOL

*2,4*-Decadien-*1*-ol.

$CH_3(CH_2)_4{-}CH{=}CH{-}CH{=}CH{-}CH_2OH$

$C_{10}H_{18}O = 154.25$

Colorless oily liquid. Very slightly soluble in water, soluble in alcohol, miscible with oils.

Oily, but fresh and citrusy odor, somewhat reminiscent of Linalool, but overall of Orange-Bitter Orange, Grapefruit-character.

Could find use in perfume compositions, mainly as a modifier in citrusy topnotes, and as a new, refreshing item to accompany certain floral fragrances in their topnote.

Suggested for use in flavor compositions, as a fortifier in Orange-Grapefruit compositions, etc. and generally in fruit imitation flavors.

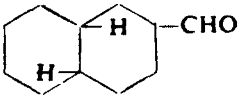
NOTE: This material is not yet approved for food use in the U.S.A. (1967).

Prod.: by selective reduction (Ponnford) of *2,4*-Decadien-*1*-al.

34-579;

## 823: **DECAHYDRO**-beta-**NAPHTHALDEHYDE**

Exists in *cis*- and *trans*-form.
Commercial material is mostly *trans*-isomer.



$C_{11}H_{18}O = 166.27$

Colorless oily liquid. B.P. 233° C.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar dry, musty, powerful odor, reminiscent of certain notes in Ambergris.

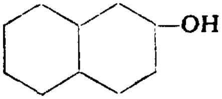
Used in perfume compositions to support Ambergris-notes, natural or synthetic.

Prod. from *beta*-Decalone with Sodium and Ethyl chloroacetate followed by saponification of the glycidate.

5-324; 86-40;

## 824: trans-**DECAHYDRO**-beta-**NAPHTHOL**

*trans-beta*-Decanol.
(sometimes called "Decalinol").
Bicyclo-*4,4,0*-Decanol.



$C_{10}H_{18}O = 154.25$

Colorless viscous liquid, solidifying in the cold to an opaque mass. The presence of variable amounts of the *cis*-isomer is mainly responsible for the variations in physical appearance of this material.

Mild, sweet, slightly camphoraceous-woody, also warm and mildly spicy odor of fair tenacity. The odor has been compared to that of Dihydrocarveol, but such description does not help many perfumers.

Practically insoluble in water, soluble in alcohol and oils.

This alcohol has been used, and is still used on a modest scale, in perfume compositions, mostly in connection with woody and camphoraceous fragrance types, including the Ionones, Cyclohexylderivatives, etc. Several of its esters (see following monographs) have been more successful as perfume materials).

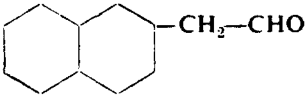
However, since the Ambregris- and Sandalwood-notes, which are represented to a certain degree in the esters, can be obtained with much superior beauty by way of modern perfume chemicals, there is reason to believe that the Decahydronaphthyl series will eventually become obsolete.

Prod.: by catalytic hydrogenation of *beta*-Naphthol. The reaction yields a mixture of *cis*- and *trans*-isomers, but the perfumers generally prefer the *trans*-isomer, or a material primarily consisting of that isomer.

4-40; 86-40;

## 825: **DECAHYDRO**-beta-**NAPHTHYLACETALDEHYDE**

Decalylethanal.
Occasionally confused with:
Decahydronaphthaldehyde (see earlier monograph).
or: Tetrahydro naphthylacetaldehyde (see monograph).



$C_{12}H_{20}O = 180.29$

Colorless oily liquid. B.P. 236° C.

Insoluble in water, soluble in alcohol and oils.

Semi-dry, musty-woody odor with a remote resemblance to notes in Ambergris. However, the olfactory picture is very incomplete and the tenacity very poor – compared to Ambergris products.

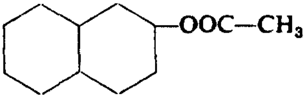
The author believes that this material has little or no interest to the perfume industry, but it is included in this work to complete the monographs on the Decahydronaphthol-series, and to briefly describe products which may be used on a small scale in perfumery.

Prod.: by oxidation of *beta*-Decalyl ethanol.

Also from Decahydro naphthaldehyde via the glycidic ester to the subject material.

## 826: trans-**DECAHYDRO**-beta-**NAPHTHYL ACETATE**

"Decalinyl acetate".
"Jasmalol".
– and other trade names.



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. B.P. 200° C. Sp.Gr. 0.92.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-fruity, slightly oily and floral odor of Jasmin type. The odor has been compared to that of Benzylacetate with a "hydrocarbon" note, but the author finds that a good grade of the subject ester does not display hydrocarbon-like notes. In spite of its boiling point being very close to that of Benzylacetate, the subject ester gives impression of being much less volatile. It has no pungency, but no freshness either, in its immediate odor picture. In fact, it does outlast Benzylacetate on a blotter test, but one is inclined to find more "power" in Benzylacetate.

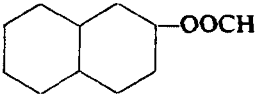
In any event, the material has found its way into perfume compositions where it enjoys a modest popularity as a variant among the fruity Jasmin base materials, a modifier of the Benzyl family, and a smaller ingredient in Gardenia and other floral fragrances. Its relatively low cost (not nearly as low as Benzylacetate) makes it useful in ordinary fragrances for household products, etc. industrial odors, masking odors, etc.

Prod.: by acetylation of *trans*-Decahydro-*beta*-naphthol (see earlier monograph).

4-41; 3-37; 33-504; 86-40; 155-98;

## 827: **DECAHYDRO**-beta-**NAPHTHYLFORMATE**

"Santiat".
"Santalozon".
"Violaron".
*beta*-Decalinyl formate.



$C_{11}H_{18}O_2 = 182.27$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Sweet-woody, musty and slightly green odor of moderate tenacity. The Sandalwood-like notes, for which this ester is still appreciated, appear most conspicuously in dilutions of less than 10% of this ester with significant amounts of mild, sweet and woody blenders.

In itself, it displays a rather herbal and root-like character, not immediately reminiscent of any typical note from Sandalwood.

The ester is still used in perfume compositions as component of Sandalwood bases, in woody and Ambre-like fragrances, and very often in combination with the Ionones or Methylionones. That combination produces quite attractive notes.

In view of the newer Sandalwood-smelling chemicals developed and made available since the late 1950's, there is probably not much future for the subject ester, except in already established formulations many of which have been quite successful.

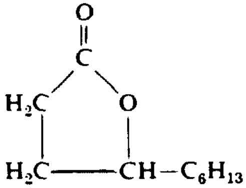
It is interesting to note that the Decahydro naphthyl series was originally brought into the market by a very large chemical company, not specializing in perfume chemicals. That same company is now making Linaool and related perfume chemicals available at very attractive cost by way of interesting new syntheses.

Prod.: by formylation of *beta*-Decalinol. The commercial product will inevitably contain two stereo-isomer forms of subject material.

3-36; 3-114; 4-41; 4-128; 4-40; 86-122;

## 828: gamma-n-**DECALACTONE**

*gamma-n*-Hexyl-*gamma*-butyrolactone.
Decanolide-*1,4*.
"Peachtone" (Dodge & Oleott).



$C_{10}H_{18}O_2 = 170.25$

Colorless oily liquid. B.P. 281° C.
Sp.Gr. 0.95.

Almost insoluble in water, soluble in alcohol and oils.

Refined, oily-peachy and extraordinarily tenacious odor. More Peach-like, less Nut-like than Nonanolide-*1,4*.

Very powerful, creamy-fruity, Peach-like taste in concentrations below 5 ppm, perceptible well below 0.2 ppm.

This Lactone is considered superior to Nonalactone ("Aldehyde C-18") and Undecalactone ("Aldehyde C-14") as a flavor material, and if it is of proper quality, it shows excellent versatility as a modifier for both of the named Lactones, advantageously substituting for part of one or both in combination fruit flavors, where Peach is the main theme, or where delicately fruity notes are desirable with sweet, mildly Nut-like or oily-creamy flavor types.

The Lactone exists in several isomers, at least three of them being commercially available. One isomer is mentioned in this work under the name: *alpha-n*-Hexyl-*gamma*-butyrolactone.

It finds use in floral perfume compositions, particularly those of Gardenia and other heavy floral type, and often in combination with considerable amounts of synthetic musks.

Its main use is, however, in flavor compositions, Peach, Mango, Strawberry, Chocolate, etc. while its use in Milk, Cream, Butter and Cheese compositions is largely abandoned in favor of the use of the *delta*-Decalactone (see next monograph).

Concentrations are usually very low, mostly less than 1 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2360.

Approved by the American FDA for use in food flavors.

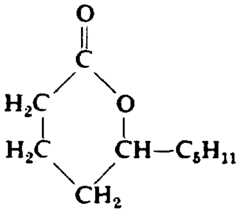
Prod.:

1) from Hexyl ethylene oxide and Sodiomalonic ester.
2) by Lactonization of Decenoic acid.

31-172; 86-40; 86-81; 156-226;

## 829: delta-DECALACTONE

Decanolide-*1,5*.
Amyl-*delta*-valerolactone.



$C_{10}H_{18}O_2$ = 170.25

Colorless viscous liquid. Almost insoluble in water, soluble in alcohol and oils.
Sp.Gr. 0.97.

Very powerful and very tenacious, sweet creamy, Nut-like odor with a heavy fruity undertone. The undiluted material displays a rather coumarinic sharpness in its topnote, but at concentrations of 0.1% or lower, it seems to grow in volume, sweetness and oily-creamy softness.

The taste is creamy, sweet Coconut-Peach-Milk-like in concentrations below 2 ppm. Minimum perceptible is well below 0.1 ppm, which puts the subject material in the class of very powerful flavor chemicals.

Blending the material with *gamma*-Decalactone and *delta*-Dodecalactone will often result in a distinct increase in the acceptability of this flavor. The "Mushroom-like" notes in the subject Lactone are subdued not only by dilution, but also by blending with the isomers and homologues.

This Lactone – only recently made commercially available – is used on a small scale in perfume compositions, often as part of a new musky type fragrance, or as a modifier in heavy floral fragrances where other Lactones are already employed (Gardenia, Tuberose, etc.).

Its main use and original purpose was that of a Milk and Cream flavor re-conditioner. It is now used on an increasing scale in Oleomargarine where its flavor comes to full bloom in combination with *delta*-Dodecalactone. In such "oily" products, actually performing a fixation upon the flavor chemical, it is necessary to use a higher concentration, and the Food authorities have realized this in permitting up to 10 ppm of this Lactone in Oleomargarine. Much lower concentrations are used in other food products.

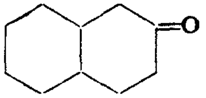
G.R.A.S. F.E.M.A. No.2361 approved by the FDA. (Use in Oleomargarine limited).

Prod.: (many methods) e. g. from Amyl cyclopentanone via *5*-Hydroxydecylic acid, by Lactonization to subject material.

157-306; 158-106; 31-174; 162-615;
(Sample and data: Soda Aromatic Co., Ltd. Japan).

## 830: beta-DECALONE

Decahydro naphthalone.
The commercial products consist of a mixture of *cis*- and *trans*-isomers.



$C_{10}H_{16}O$ = 152.24

Viscous colorless liquid, solidifying in the cold.

Practically insoluble in water, soluble in alcohol and oils.

The *cis*-isomer is liquid and boils at 247° C.

The *trans*-isomer is solid below 6° C. and boils at 241° C.

Semi-dry, tenacious odor resembling part of the Ambregris-picture, also woody, remotely reminiscent of Sandalwood. Odor variations are observed in materials from different sources of supply.

This ketone has found a little use in perfume compositions, including soap perfumes, where it can introduce pleasant background notes in support of Musk Ambrette, Labdanum, Methylionones, etc.

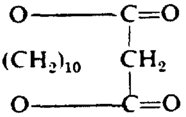
Recent development in Ambregris chemicals has brought much superior materials in the hands of the perfumer, and it is very likely that the title material, and many of its relatives, will become obsolete within the next decade or so.

Prod.: by oxidation of *beta*-Decalol with Chromic acid mixture.

67-323; 67-327;

## 831: DECAMETHYLENE MALONATE

Decamethylene glycol, Propanedioic ester (cyclic).



$C_{13}H_{22}O_4$ = 242.32

Colorless viscous oil, solidifying in the cold.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet and faintly musky odor of considerable tenacity.

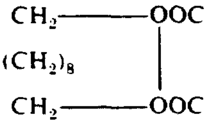
This cyclic ester had some mission at the time of its development, since it was a low-cost, non-Nitro musk of good solubility. However, newer musks have been developed in such number and at all price levels, power levels and odor types, that these original cyclic esters, with a few exceptions, have lost their importance in perfumery. It is reasonable to state that this ester now has little more than academic interest.

Prod.: from Decamethylene glycol and Malonic acid.

30-273; 31-129; 159-440;

## 832: DECAMETHYLENE OXALATE

Decamethylene glycol ethanedioic ester (cyclic).



$C_{12}H_{20}O_4$ = 238.29

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and rather fresh, musky odor of good tenacity.

The comments on this ester would be very much the same as for Decamethylene malonate (see previous monograph). However, it is fair to say that this ester has a more pleasant, almost refreshing musky odor than most of the other cyclic esters. It lacks power, and could not compete with the Ethylene brassylate or with the newer macrocyclic musks, some of which are produced at very attractive cost.

Prod.: from Decamethylene glycol plus Oxalic acid.

30-273; 31-129; 159-440;

## 833: n-DECANAL

Aldehyde C-10.  
*n*-Decyl aldehyde.  
Capric aldehyde.  
Capraldehyde.  
Caprin aldehyde.

$CH_3(CH_2)_8CHO$

$C_{10}H_{20}O$ = 156.27

Colorless, slightly oily liquid. Sp.Gr. 0.85. B.P. 209° C.

Very slightly soluble in water, soluble in alcohol, miscible with oils.

Penetrating and very powerful, sweet-waxy, Orange-peel-like odor. In extreme dilution refreshing, Citrus-peel-like.

The flavor of this aldehyde is pleasant only at concentrations well below 5 ppm. Consumer products usually contain much less than 5 ppm of the aldehyde.

Extensively used in perfume compositions, although always in low percentage, mostly less than 1 % of the total base or formulation. Distinctly aldehydic bases may, naturally, contain much more of the aldehyde.

Excellent for Citrus topnotes, for Neroli, Rose, Jasmin, Violet, Acacia, etc. and blends well with Linalool and related alcohols, Cyclamal and other floral aldehydes, and combines pleasantly with the conventional alifatic aldehydes.

It is extremely important for finer perfumery work that this aldehyde is free from traces of acid, Octanal or other lower aldehydes, etc.

Prod. from *n*-Decanol by catalytic oxidation.

G.R.A.S. F.E.M.A. No.2362.

5-80; 26-448; 77-202; 89-28; 103-207; 106-35; 128-108; 156-19; 156-22; 156-23; B-I-711; 140-158;

## 834: DECANAL DIETHYL ACETAL

*n*-Decylaldehyde diethylacetal.
*1,1*-Diethoxy decane.

$CH_3(CH_2)_8CH(OC_2H_5)_2$

$C_{14}H_{30}O_2 = 230.39$

Colorless liquid. B.P. 241° C.

Very slightly soluble in water, soluble in alcohol and oils.

Fresh-citrusy, green-oily odor with more or less pronounced aldehydic undertone, according to the chemical purity of the Acetal. The presence of only 2-3% free Aldehyde is sufficient to overcome the characteristic odor of the Acetal.

The Acetal finds some use in flavor compositions, mainly of the Citrus type, Brandy, Cognac, Liqueur, etc. and the concentration is usually mere traces in the finished product.

Prod.: from Decanal and Ethyl alcohol by condensation.

5-318; 140-159;

## 835: DECANAL DIMETHYL ACETAL

*10,10*-Dimethoxy decane.
Decylaldehyde DMA.
Capraldehyde DMA.

$CH_3(CH_2)_8CH(OCH_3)_2$

$C_{12}H_{26}O_2 = 202.34$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Green-fruity, Citrus-waxy odor.

Finds some use in perfume compositions, mainly in heavy floral bases, Gardenia, Cassie, Tuberose, etc. and occasionally in Citrusy topnotes as a modifier for the Aldehydes. Its odor is overall more refreshing than that of the parent aldehyde.

Traces of the Acetal are used in various flavor compositions, e. g. imitation Brandy, Cognac, Liqueur, and in Citrus flavors.

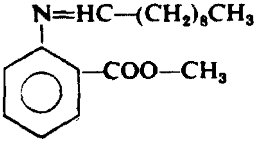
G.R.A.S. F.E.M.A. No.2363.

Prod. from Decanal and Methyl alcohol by condensation.

37-281;

## 836: DECANAL-METHYLANTHRANILATE

A "Schiff's base" type of condensation product. "Decylique" (Fritzsche Bros. Co.).



$C_{18}H_{27}NO_2 = 289.42$

Intensely yellow, somewhat viscous liquid. Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Powerful odor, mainly of Orangeblossom-type, overall floral, but with perceptible notes from the parent materials. Very tenacious.

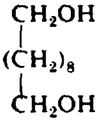
Useful in perfume compositions for heavy floral types, such as Orangeblossom, Honeysuckle, Magnolia, etc. and, in general as a floralizer and sweetener.

Prod.: by condensation of Methylanthranilate with Decanal.

(Fritzsche Bros. data.).

## 837: DECANE DIOL

*1,10*-Decanediol.
Decamethylene glycol.



$$\begin{array}{l} CH_2OH \\ | \\ (CH_2)_8 \\ | \\ CH_2OH \end{array}$$

$C_{10}H_{22}O_2 = 174.29$

Crystal needles. M.P. 74° C. B.P. 290° C.

Practically insoluble in water. Soluble in alcohol and oils.

Very faint, sweet-musty odor.

Bland taste.

Of very little use as such (mostly a diluent/solvent), this chemical is an important intermediate in the manufacture of many perfume chemicals. It occurs in trace amounts in many end products.

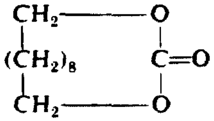
Its high boiling point has given it some use as a mild fixative in perfume compositions. Nitromusks and Indane musks seem to benefit from blending with this Glycol.

Prod.: by reduction of Diethyl sebacate with Sodium ethylate, or: by hydrogenation of Diethyl sebacate under high pressure.

100-322;

## 838: 1,10-DECANEDIOL CARBONATE

Decamethylene glycol carbonate.
Decamethylene carbonate.



$C_{11}H_{20}O_3 = 200.28$

Colorless viscous liquid, solidifying in the cold.

Almost insoluble in water, soluble in alcohol and oils.

Woody-camphoraceous, but also floral odor of good tenacity. The odor may appear sweet to some observers, rather dry to others. It is conceivable that the commercial material, only occasionally offered, is not a pure, single chemical.

This material has been used in perfume compositions where woody and rosy notes are combined, e. g. in modern soap perfumes, and it also blends well with Lavender, Ionones, Lavandin, Rosemary, Cyclohexane-derivatives, etc.

Prod.:

1) from Decamethylene glycol and Carbonylchloride (= Phosgen).
2) from Decamethylene glycol and Diethylcarbonate by cross-esterification with a Sodium catalyst. The resulting high-polymer product is subsequently depolymerized. Purification via boration to remove last traces of Glycol.

159-439;
(See also: 31-127; and 30-272;)

## 839: DECANE NITRILE

Decyl cyanide.
Undecyl nitrile.

$CH_3(CH_2)_8CH_2—CN$

$C_{11}H_{21}N = 167.30$

B.P. 254° C.
Colorless liquid, slightly soluble in water, soluble in alcohol and oils. Decomposes in acid aqueous media, but is comparatively stable in alkali.

Powerful, somewhat musty-fatty, Walnut-like odor, with a vague resemblance to alifatic Aldehydes in its diffusive power and radiant odor.

Has been suggested for use in perfume compositions, e. g. where the alkalinity in the functional product may cause decomposition of aldehydic components of similar odor.

Together with many related Nitriles, this chemical has generally failed to attain popularity among the creative perfumers. One of the first Nitriles in this series to be commercially produced was the Nitrile of Myristic acid, developed by Dr. Georges Igolen in the early 1950's, in Grasse (Antoine Chiris). There still seems to be some doubt (or maybe fear??) that these chemicals may be accompanied with a hazard of producing trace amounts of Hydrocyanic acid. This should virtually be out of the question in case of absolutely pure chemicals.

Prod.: From Decyl bromide plus Sodium cyanide.

26-714; B-II-358;

## 840: DECANOIC ACID

Capric acid.
Decylic acid.
Nonanecarbonic acid-*1*.

$CH_3(CH_2)_8COOH$

$C_{10}H_{20}O_2 = 172.27$

Colorless needles or translucent crystalline mass. M.P. 31° C. Sp.Gr. 0.89 (liquid).
B.P. 270° C.

0.015% soluble in water, soluble in alcohol and oils.

Rather unpleasant, sour-fatty, "rancid" odor.

Finds very little, if any, use in perfume compositions, perhaps occasionally in the reconstruction of certain essential oils.

Used in flavor compositions, mainly in imitation Butter, Cheese, Coconut, Fruit, Liqueur, Rum, Whisky, etc.

Concentration in the functional product is normally just traces.

Prod.: by oxidation of Decanol (obtained from Coconut oil or otherwise).

G.R.A.S. F.E.M.A. No.2364.

26-448; 66-564; 100-205; B-II-355; 90-94;-77-187; 140-143;

## 841: DECANOL-1

*1*-Decanol.
*n*-Decyl alcohol.
Alcohol C-10.
Decylic alcohol.
"Capric alcohol".
Nonyl carbinol.
"Lorol No.22" (DuPont) is mainly Decanol.

$CH_3(CH_2)_8CH_2OH$

$C_{10}H_{22}O = 158.29$

Colorless liquid, solidifies in the cold.
M.P. 7° C. B.P. 233° C. Sp.Gr. 0.83.

Insoluble in water, soluble in alcohol and oils.

Sweet, slightly fatty-oily odor, waxy and floral, mainly rosy, also reminiscent of Lily and Orangeblossom, but fresher, in the same way as Citronellol is fresh.

The taste is floral, oily, mainly citrusy.

Widely used in perfume compositions,

although often only in traces. More liberally used in masking odors for industrial purposes, – and as a blender, modifier for Linalool, Citronellol, etc. in low-cost floral blends. It blends well with the alifatic Aldehydes and lends softness to these.

Used in flavor compositions, mainly in imitation Butter, Orange, Coconut, Lemon and various combination fruit flavor types.

Concentration in the finished consumer product is normally mere traces.

G.R.A.S. F.E.M.A. No.2365.

Prod.: by fractionation of Coconut fatty alcohols isolated via esterification and reduction.

5-15; 26-472; 41-24; 44-806; 77-172; 100-322; 140-125; 106-28; B-I-425;

## 842: DECEN-2-AL

*2*-Decenal.
Decenaldehyde.
Decylenic aldehyde.
(trans-isomer is of commercial interest).
*beta-n*-Heptylacralein.
*3*-Heptylacrolein.

$CH_3(CH_2)_6—CH=CH—CHO$

$C_{10}H_{18}O = 154.25$

Colorless oily liquid. B.P. 229° C.
Sp.Gr. 0.84.

Insoluble in water, soluble in alcohol and oils.

Very powerful, waxy-Orange-like, sweet-"aldehydic" odor of fair tenacity and high diffusive power.

Finds occasionally some application in perfume compositions, mainly in the reconstruction of certain essential oils, or as an additive to Citrus bases for topnote effects.

Used in fruit flavors, mainly Citrus types, but also in Peach, Apricot and other fruit flavors, where it may introduce a fresh-green note.

G.R.A.S. F.E.M.A. No.2366.

Prod.: from *alpha*-Bromocapric acid via Decenoic acid and its Ethylester to Decenol, which is oxidized to Decenal.

Also produced from Acetaldehyde by condensation with *n*-Octanal.

(156-26); 4-59; 89-47;
(sample: Compagnie Parento, Inc.).

## 843: 2-DECENOIC ACID

*3*-Heptyl acrylic acid.
*2*-Decylenic acid.
The *trans*-isomer is most common in Nature, and it occurs often together with *cis-4*-Decenoic acid.
9-Decenoic acid occurs in Milk- and Butter fat.

$CH_3(CH_2)_6CH=CH—COOH$

$C_{10}H_{18}O_2 = 170.25$

Colorless liquid, solidifying in the cold to a waxy, opaque mass. Practically insoluble in water, soluble in alcohol and oils.

Powerful, waxy-harsh odor when undiluted, almost Stearin-like unpleasant fatty. Sweet, refreshingly fruity and slightly oily-waxy in concentrations lower than 0.1 %. Poor tenacity.

The taste in concentrations lower than 5 ppm is fruity, slightly waxy but sweet and Peach-Orange-like.

This acid has found some use in the reconditioning of flavor in processed fruit, Orange and Peach in particular. It is often used in conjunction with *2*-Dodecenoic acid, and both materials are kept at concentrations of a few ppm in the finished product, sometimes even lower.

Although this acid has not been recommended for use in perfume compositions, there could be some use for it in Citrus bases, particularly Orange, Bitter Orange and Grapefruit.

Prod.:

1) from *beta*-Hydroxydecanoic acid by dehydration.
2) by oxidation of Decen-*2*-ol-*1* with Potassium dichromate and diluted sulfuric acid to obtain the aldehyde, from which the acid can be obtained by ozonization.

## 844: omega-DECENOL

"Rosalva" (I.F. & F.).
*9*-Decenol-*1*.
Decylenic alcohol.
"Rosal" (Alpine Aromatics).

$CH_2{=}CH(CH_2)_7{-}CH_2OH$

$C_{10}H_{20}O = 156.27$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, fatty-oily, waxy-rosy odor of considerable tenacity. The rosy notes are particularly conspicuous in dilutions, best at 1% or lower, while higher concentrations bring about more waxy-oily notes.

This alcohol, simple from a chemical point of view, has achieved much popularity since it was originally introduced in the late 1950's. Its stability in soap (perfumes) and its immense power and floral radiation, particularly when blended with alifatic aldehydes, was quickly utilized in very successful and world-wide known soap fragrances.

Its success in soap perfumes apparently gave the perfumers the impression that this was a "soap perfume chemical" and the alcohol was only rarely used in other fragrances. Yet, smaller amounts find their way into a multitude of floral and refreshing, sweet fragrance types, and in modern detergent fragrances as well. Although basically a Rose material, it is not confined to typically rosy odors, in fact, it can be used as a "lifting" material in conjunction with *iso*-Butylquinoline and Ionones, and it gives interesting effects with Styrax materials.

As the patent by which this alcohol is manufactured is expiring, one might expect a flood of material coming on the market at lower cost, but it is most unlikely that this material will be manufactured by any great number of companies. It is not as easy as one should think to achieve the odor purity, and it is not easy to manufacture the alcohol on a large scale.

In its effect and overall type, it bears some similarity to the higher, and branched-chain, alifatic aldehydes, e. g. Norhexahydrofarnesal, etc.

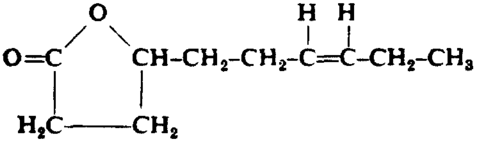
Prod.: from Decamethylene glycol.

I.F.F. sample.

34-579; (see also Chemical Week, Nov. 1961).

## 845: 7-DECENOLACTONE

*gamma-3*-Decenolactone (misleading name).
*gamma-3*-Hexenyl butyrolactone.



$C_{10}H_{16}O_2 = 168.24$

Almost colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and very diffusive, fatty-buttery, oily-Nut-like odor of considerable tenacity. Sweeter and less fatty than Decalactone. Powerful oily-buttery, somewhat fatty and green-nutty taste in dilutions below 1 ppm.

This Lactone, rarely offered commercially, has been suggested for use in flavor compositions as part of the powerful and natural notes in imitation Butter, Cream, Nut, Milk, and similar flavor types. It would be used at the concentration of less than 1 ppm calculated on the finished consumer product.

The material is NOT yet listed as G.R.A.S. in the American Federal Register of Food Chemicals.

It could undoubtedly find good use in perfume compositions to lend the often desirable "creamy" topnote to certain floral types, and it would also be useful in the reconstruction of certain flower absolutes as part of the waxy "petal" notes.

Prod.: From Ethyl allyl malonic ester via its aldehyde to Succinic semialdehyde which is reacted with Hexenyl magnesium chloride to yield the Lactone.

31-175; 86-81; 4-61; 86-41;

## 846: DECENYL ACETATE

9-Decen-*l*-yl acetate.
"Roseate" (I.F.&F.).

$CH_2{=}CH(CH_2)_7{-}CH_2{-}OOC{-}CH_3$

$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Pleasant, oily-rosy, Rose-petal-like odor of considerable diffusive power and tenacity.

Finds some use in perfume compositions as a modifier for fresh-floral and aldehydic fragrance materials, as part of the topnote base in Rose and other florals, Peony compositions, Magnolia, etc.

Prod.: by direct esterification of *omega*-Decenol, "Rosalva" (I.F.&F.).

## 847: DECENYL PROPIONATE

9-Decen-*l*-yl propionate.

$CH_2{=}CH(CH_2)_7CH_2{-}OOC{-}CH_2{-}CH_3$

$C_{13}H_{24}O_2 = 212.34$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Delicately floral-oily, sweet and slightly fruity odor with rosy overtones and a soft, but tenacious Ambrette-seed-like background.

Finds some use in perfume compositions, mainly as a modifier in topnote compositions of floral or aldehydic character. It imparts interesting effects to Muguet, Rose, Lily, Cyclamen and Citrus compositions, and it introduces a pleasant freshness in Ambre-bases.

Prod.: by direct esterification of 9-Decenol with Propionic acid, e. g. under azeotropic conditions, or with Propionic anhydride.

## 848: DECYL ACETATE

"Acetate C-10".
Decanyl acetate.

$CH_3(CH_2)_8CH_2{-}OOC{-}CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. B.P. 244° C.

Insoluble in water, soluble in alcohol and oils.

Sweet fatty-fruity odor of Pineapple-Orange-like character, and rosy waxy undertones.

Finds a little use in perfume compositions as a modifier for Linalyl acetate, and generally as a "fresh" note in delicate florals (Muguet, etc.) or in aldehydic topnote compositions. It blends excellently with Dodecanal (Aldehyde C-12, Lauric).

Finds some use in flavor compositions,

mainly for imitation Apple, Berry, Honey, Orange, Peach, Plum, etc. and also in Rum flavors. The concentration of Decyl acetate in the functional product amounts usually to traces only.

G.R.A.S. F.E.M.A. No.2367.

Prod.: by direct esterification of *n*-Decanol with Acetic acid under azeotropic conditions – or with Acetic anhydride.

26-472; 31-122; 43-504; B-II-135; 86-41; 4-41; 77-182; 140-135;

## 849: iso-DECYL ACETATE

A mixture of isomers,
mainly: Methyl-*n*-nonylacetate.
The above name is also used for:
*2,6*-Dimethyl octanylacetate.

$$C_{12}H_{24}O_2 = 200.32$$

Colorless liquid, almost insoluble in water, miscible with alcohol and oils.

Fresh-citrusy, rosy-sweet odor, somewhat reminiscent of Linalyl acetate, not quite as sweet, and rather fresher.

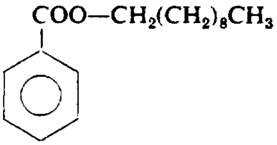
Has been suggested for use in perfume compositions, including soap perfumes as a modifier for Linalyl acetate in citrusy compositions. The ester had some mission when Linalyl acetate was comparatively expensive (up until 1958), but it has lost its foothold on the perfumer's shelf ever since.

Could find some use in flavor compositions, but does not really offer any unusual effects or flavor types.

Prod.: from *iso*-Decanol by direct esterification with Acetic anhydride plus Sodium acetate. or: from Tripropylene by Acetylation. The Oxoalcohol is subsequently esterified.

31-122;

## 850: DECYL BENZOATE



$$C_{17}H_{26}O_2 = 262.40$$

Almost colorless, viscous liquid.

Insoluble in water, soluble in alcohol, poorly soluble in Propylene glycol, miscible with oils.

Sp.Gr. 0.96. B.P. 305° C.

Very tenacious, but comparatively mild, herbaceous-earthy odor with a musky note. It bears an overall resemblance to the odor of certain garden herbs and condiments in its sweet-balsamic character.

Has been suggested for use in perfume compositions, but is rarely applied, although commercially available. It could give interesting effects in new types of "Oriental" fragrances, and it blends well with Cinnamic alcohol, Sandalwood oil, the various Rose alcohols, etc.

Prod.: by direct esterification of *n*-Decanol with Benzoic acid under azeotropic conditions.

35-854; 86-41;

## 851: DECYL BUTYRATE

Decanyl butyrate.

$CH_3(CH_2)_8CH_2—OOC(CH_2)_2CH_3$

$$C_{14}H_{28}O_2 = 228.38$$

Colorless, slightly oily liquid. Insoluble in water, soluble in alcohol and oils.

B.P. 270° C. Sp.Gr. 0.89.

Mild-fruity, somewhat Brandy-like, Apricot-type odor.

Sweet, oily-fruity, Apricot-like taste with a slightly floral note. In spite of apparent power, its taste is rather bland, nondescript fruity. Finds little or no use in perfumery.

Used in flavor compositions, mainly in Apricot, Peach and other fruit bases, in Citrus flavors, etc.

Concentration is normally only traces in the finished product.

Prod.: by direct esterification of Decanol with Butyric acid, e. g. under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2368.

35-851; 140-139;

## 852: **DECYL**-iso-**BUTYRATE**

Decanyl-*iso*-butanoate.

$CH_3(CH_2)_8CH_2—OOC—CH(CH_3)_2$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, oily-herbaceous odor of good tenacity.

This relatively rare ester finds use in perfume compositions, flower bases and certain specialties. In Rose and Jasmin, it may help introduce part of the oily-waxy "petal"-like note, so often wanted, and just as often missing. Tuberose, Magnolia, Gardenia, Peony, Freesia, etc. may also benefit from this ester in trace amounts.

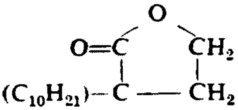
The real pleasure is to use the ester (and many other perfume materials) in quite "unconventional" places. This is where the truly interesting effect may come about.

In Lavender, perhaps along with Coriander, this ester can produce very intriguing notes, and it has equally good effects upon Ylang-Ylang and Labdanum. It represents just one more example of the wealth of possibilities at hand for the truly imaginative and daring perfumer.

Prod.: by direct esterification of *n*-Decanol with *iso*-Butyric acid under azeotropic conditions, - or with *iso*-Butyric anhydride.

## 853: alpha-n-**DECYL**-gamma-**BUTYROLACTONE**

Tetradecanolide (*1,4*).



$C_{14}H_{26}O_2 = 226.36$

Almost colorless, viscous liquid.

Practically insoluble in water, soluble in alcohol, miscible with oils.

Fresh-unctuous odor with Coconut-musky undertones.

Rarely used in perfumery.

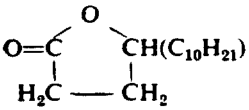
Finds a little use in flavor compositions, mainly as a modifier for Coconut and Nut flavors, Butter, Milk and Ice cream flavor compositions, etc.

Prod.: several methods, e. g.: from Ethylene oxide by *n*-Decyl malonic ester synthesis.

31-170; 156-229;

## 854: gamma-n-**DECYL**-gamma-**BUTYROLACTONE**

*gamma*-Tetradecalactone.



$C_{14}H_{26}O_2 = 226.36$

Colorless viscous oil.

Insoluble in water, soluble in alcohol, miscible with oils.

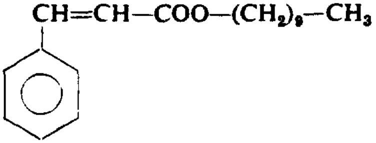
Weak, oily, sweet-fatty, remotely fruity and very tenacious odor.

Has been suggested as a modifier-fixative for perfume compositions, but has not succeeded in competition with the more powerful and characteristic smelling Lactones.

Prod. from Decyl ethylene oxide and Sodiomalonic ester. Epoxydecane is made from Decane and Perbenzoic acid in Chloroform solution.

156-229; see also: 31-172;

## 855: DECYLCINNAMATE



$C_{19}H_{28}O_2 = 288.43$

Colorless oily liquid. B.P. 338° C.

Solidifies in the cold, melts at $-7°$ C.

Has some tendency to polymerize, the liquid becoming very viscous, hazy, and almost odorless.

Oily-herbaceous, sweet odor with some resemblance to Opopanax and Heracleum fruits ("Bear's claw" fruits).

Could find some use in perfumery, particularly in Oriental compositions, where it would be a pleasant modifier to the sweet woods, balsams and mild spices.

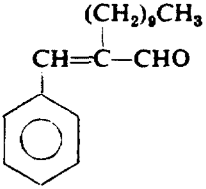
However, it is rarely offered commercially and therefore not often found on the perfumer's shelf.

Prod.: by azeotropic esterification of Decyl alcohol with Cinnamic acid, using a catalyst starter.

86-41;

## 856: alpha-n-DECYL CINNAMIC ALDEHYDE

Decyl cinnamal.



$C_{19}H_{28}O = 272.43$

Pale yellowish oily liquid. Practically insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Almost odorless when pure, but is capable of introducing pleasant oily-herbaceous and very tenacious notes in compositions.

Its effect is rather mild and weak, and does not appear very unusual. Its price is considerably higher than that of the conventional substituted Cinnamic aldehydes.

In brief, this material has little, if any, interest to the working perfumer.

Prod.: from Benzaldehyde and Dodecanal (Lauric aldehyde) by condensation.

31-51;

## 857: DECYL CROTONATE

Decyl-*trans*-crotonate.
Decyl-*alpha*-crotonate.
Decyl-2-butenoate.

$C_{10}H_{21}—OOC—CH{=}CH—CH_3$

$C_{14}H_{26}O_2 = 226.36$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Mild, oily-ethereal, faintly herbaceous odor of good tenacity.

This ester find some use in perfume compositions, especially in herbaceous fragrances, where a warm, mild background note is desirable, e. g. in Lavender-Chypres, along with Oakmoss and Opopanax, etc. but also under distinctly floral fragrances, as a "natural" mellow note in Lily, Rose, etc.

It performs very well as a companion to Coriander in modern "fantasy" type fragrances.

Prod.: by direct esterification of *n*-Decanol with *2*-Butenoic acid (*trans*-Crotonic acid).

## 858: DECYL ETHER

$CH_3(CH_2)_8CH_2-O-CH_2(CH_2)_8CH_3$

$C_{20}H_{42}O = 298.56$

Colorless liquid, insoluble in water, soluble in alcohol, miscible with oils.

Faint, oily-rosy odor of considerable tenacity. The odor of the undiluted material is not really pleasant, but the effect of the Decylether in perfume compositions can be quite attractive.

Has been suggested for use in soap perfume compositions mainly those of floral type. It introduces a soft background and lends tenacity to the composition. However, the odor value of the material is very modest, and the overall type is rather uninteresting.

Prod. from Decanol by dehydration e. g. with conc. sulfuric acid.

## 859: DECYL FORMATE

Decyl methanoate.

$CH_3(CH_2)_8CH_2—OOCH$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.

B.P. 240° C. Sp.Gr. 0.87.

Light, fruity, almost sharp odor with floral, Honeysuckle-Orangeblossom character. Its floral notes are accompanied by a heavy proportion of leafy, deep-green notes.

Interesting for Orangeblossom, Neroli, Violet, Rose and, in general as a modifier in heavy floral or Oriental fragrance types. It blends very well with Opopanax, Sandalwood, Rose materials, Ionones and Citrus oils. For Orris bases it lends the fresh-oily notes that help change Ionones into more "orrisy" notes.

Occasionally used in flavor compositions for imitation Cherry, Plum, Raspberry, Orange, etc.

Prod.: by direct esterification of Decanol with Formic acid e. g. under azeotropic conditions.

4-41; 86-61; 140-132;

## 860: DECYL OXYACETALDEHYDE

$CH_3(CH_2)_9—OCH_2—CHO$

$C_{12}H_{24}O_2 = 200.32$

Colorless viscous liquid. Practically insoluble in water, soluble in alcohol and oils.

Sp.Gr. 0.87. B.P. 238° C.

Powerful, floral-green, very diffusive, yet tenacious odor, reminiscent of Rose petals, Lily, Muguet, Peony, etc., but overall greener than the straight florals.

Interesting in perfume compositions where it may introduce desirable "waxy"-floral petal-notes in above floral types, or it may be a part of a topnote composition which can be Citrusy, floral or aldehydic. It lends power and tenacity to such materials.

Prod.: From Decanol plus Sodium Methylate. The Acetal which is formed is subsequently reacted with Bromodimethyl acetal. The resulting Acetal is finally hydrolyzed with Oxalic acid to yield the Aldehyde.

156-378;

## 861: DECYL PALMITATE

Decyl hexadecanoate.

$CH_3(CH_2)_8CH_2—OOC(CH_2)_{14}CH_3$

$C_{26}H_{52}O_2 = 396.70$

Colorless or white waxy crystalline mass, melting at low temperature to a colorless oily liquid.

Very mild, oily-waxy odor. Virtually odorless when pure.

Insoluble in water, slightly soluble in alcohol, miscible with oils. Almost insoluble in mineral oil.

This material finds a very limited use as a blender-solvent in certain perfume compositions, e. g. as an additive to flower absolutes and floral bases, in which it introduces a natural oily-waxy undertone and a general softness to the fragrance.

Prod.: by direct esterification of Decanol with Palmitic acid.

## 862: DECYL PELARGONATE

Decyl-*n*-nonanoate.
Decyl-*n*-nonylate.

$CH_3(CH_2)_8CH_2—OOC(CH_2)_7CH_3$

$C_{19}H_{38}O_2 = 298.51$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol and mineral oil.

Orange-like, oily-fruity, also floral and winey, Grape-like odor of good tenacity.

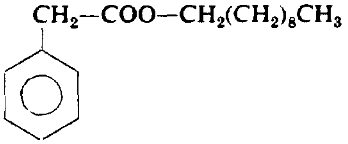
Occasionally used in perfume compositions to emphasize Grapefruit notes, Bitter Orange, etc. Also interesting as a modifier in Ambre notes.

Could find use in flavor compositions for imitation Bitter Orange, and in Citrus fruit blends.

Prod.: by direct esterification of Decanol with Nonanoic acid.

90-218;

## 863: DECYL PHENYLACETATE



$C_6H_5CH_2—COO—CH_2(CH_2)_8CH_3$

$C_{18}H_{28}O_2 = 276.42$

Colorless viscous liquid, solidifying in the cold.

Insoluble in water, soluble in alcohol, miscible with oils.

Mild, sweet and very tenacious floral odor, remotely reminiscent of Rose or Peony, but with somewhat herbaceous undertone.

Has been suggested for use in perfume compositions, where its great tenacity would place it among the fixatives, while its odor contribution is rather modest. It remains a rare chemical not commonly found on the perfumer's shelf.

Prod.: By direct esterification of Decanol with Phenylacetic acid under azeotropic conditions.

## 864: DECYL PROPIONATE

$CH_3(CH_2)_8—CH_2—OOC—C_2H_5$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid. Very slightly soluble in water, soluble in alcohol and oils.
Sp.Gr. 0.88.  B.P. 265° C.

Fatty-aldehydic, musky, sweet and pleasant odor, somewhat reminiscent of certain notes in Ambrette seed.

Finds some use in perfume compositions, partly as a topnote ingredient to support fresh-citrusy or Ambrette-seed-like notes, partly as a modifier in Citrus fragrance and fruity notes.

Used in flavor compositions for imitation Citrus fruit, other fruit and Brandy flavors.

Concentration in the finished product is normally mere traces.

G.R.A.S. F.E.M.A. No.2369.

35-854; 86-42; 103-109;

## 865: DECYL PYRUVATE

Pyroracemic acid, Decylester.

$CH_3(CH_2)_8CH_2—OOC—CO—CH_3$

$C_{13}H_{24}O_3 = 228.34$

Colorless or pale straw-colored liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-herbaceous, somewhat winey-caramellic odor of modest tenacity.

Could possibly find some use in perfumery, mainly in the creation of essential oil substitutes, etc.

Could find use in flavor compositions. Gives interesting effects in Coconut, Nut, Caramel, Rum and similar flavor types.

Prod.: By direct esterification of Decanol with Pyruvic acid.

## 866: DECYL THIOGLYCOLATE

Decyl mercapto acetate.

$CH_3(CH_2)_8CH_2—OOC—CH_2—SH$

$C_{12}H_{24}O_2S = 232.39$

Colorless, somewhat viscous liquid.
Sp.Gr. 0.95.

Almost insoluble in water, soluble in alcohol and oils.

Faint, fresh-oily odor. This could possibly be notes from traces of surplus Decanol in the ester.

In any event, this ester finds very little, if any, use in perfumery.

Prod.: directly from Decanol and Thioglycolic acid.

34-1245;

## 867: DECYL-iso-VALERATE

Decyl-*beta*-methyl butanoate.
Decyl-*beta*-methyl butyrate.

$CH_3(CH_2)_8CH_2—OOC—CH_2—CH(CH_3)_2$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid. B.P. 280° C.
Sp.Gr. 0.87.

Insoluble in water, soluble in alcohol and oils, slightly soluble in Propylene glycol.

Ethereal, oily-fruity, faintly Apple-like odor, also reminiscent of the fatty notes in Pineapple.

Sweet, oily-fruity flavor.

Finds little or no use in perfumery.

Useful in flavor compositions for imitation Apple, Arak, Brandy, Apricot, Pineapple, etc.

Prod.: by direct esterification of Decanol with *iso*-Valeric acid.

35-854;

## 868: DECYL VINYL ETHER

"Decave" (I.F. & F.).
Ethenyl oxydecane.
Vinyl decyl ether.

$CH_3(CH_2)_8CH_2—O—CH=CH_2$

$C_{12}H_{24}O = 184.32$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Refreshing, citrusy-waxy, light and floral (mainly rosy) fragrance of moderate tenacity, but good radiation. A very "clean" odor although not strikingly natural, it has notes in common with the alifatic aldehydes and the C-12 alcohols.

This ether is used in perfume compositions, particularly in soap and detergent fragrances, where its odor type is nearly perfect. It emphasizes the "soapy" clean odors, it gives lift to floral and citrusy aroma chemicals, blends excellently with Benzylacetate, Limonene, Lavender and Citrus oils, Ionones and Amylsalicylate, etc.

Being stable under alkaline conditions is just one more advantage of this chemical, and it is sufficiently inexpensive that one can use it liberally in household product fragrances.

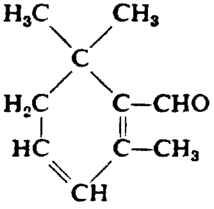
If it is used in better cosmetic perfumes, it may show quite interesting possibilities. The effect it has on Coriander oil is very intriguing, and it gives agreeable novel notes in Lime compositions, so very popular these years (1968- – ).

Prod.: from Decanol (alcohol C-10) plus Acetylene under pressure, in presence of a catalyst, usually an alkoxide.

Product sample from I.F & F. Inc.

## 869: DEHYDRO-beta-CYCLOCITRAL

Safranal.
*2,6,6*-Trimethyl-*4,4*-cyclohexadiene-*1*-carboxaldehyde.
*1,1,3*-Trimethyl-*2*-formylcyclohexadien-*2,4*.



$C_{10}H_{14}O = 150.22$

Pale yellowish oily liquid. Almost insoluble in water, soluble in alcohol and oils.
Sp.Gr. 0.97. B.P. 227° C.

Very powerful, sweet, green-floral and somewhat tobacco-herbaceous odor of good tenacity. In extreme dilution reminiscent of the odor of Safran (Saffron).

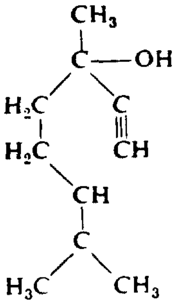
Interesting material for fresh topnotes, as a modifier for aldehydic-citrusy notes, as a green-floral topnote in flower fragrances, etc. It blends excellent with the alifatic Aldehydes, with Oakmoss products and herbaceous oils, etc.

The aldehyde is, to the author's knowledge, not used extensively in flavor compositions.

Prod.:
1) from Picrocrocin.
2) by dehydration of *beta*-Cyclocitral with Selenium dioxide.

4-127; 68-190; 89-120; 100-915;

## 870: DEHYDROLINALOOL



$C_{10}H_{16}O = 152.24$

Colorless or pale straw-colored liquid.

This chemical constitutes a trace impurity in commercial lots of synthetic Linalool (from Acetylene) and is an important intermediate in the manufacture of high-purity Linalyl esters, which are obtained by hydrogenation of the Dehydro linalylesters.

Prod.: as the last step in making Linalool by Acetylene – Acetone process. Dehydrolinalool is finally hydrogenated to Linalool. (Hoffmann-laRoche).

156-236;

## 871: DIACETIN

Glyceryl diacetyte.
*1,2*-Diacetin (mainly).

mainly: $CH_2-OOC-CH_3$
$CH-OOC-CH_3$
$CH_2-OH$

$C_7H_{12}O_5 = 156.17$

Colorless, slightly viscous liquid.
Sp.Gr. 1.18. B.P. 280° C.

Soluble in water and alcohol. Poorly soluble in most perfume and flavor oils. Miscible with Propylene glycol.

Almost odorless, or having a faint, sweet-ethereal odor.

Mainly used as a solvent in flavor compositions. Practically no use in perfumery.

In normal use-dilutions there is no perceptible flavor of this ester.

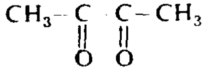
Prod.:

1) from Glycerin with 2 mol. Acetic acid.
2) from Allyl acetate with Hypoiodous acid, followed by reaction with Potassium acetate.

26-560; 66-1024; 100-332; B-II-147;

## 872: DIACETYL

Biacetyl.
*2,3*-Diketobutane.
Dimethyl glyoxal.
"Dimethylketone" (misleading name).
*2,3*-Butane dione.



$CH_3-\underset{\underset{O}{\|}}{C}-\underset{\underset{O}{\|}}{C}-CH_3$

$C_4H_6O_2 = 86.09$

Intensely yellowish or greenish-yellow mobile liquid. Solidifies in the cold. M.P. minus 3° C. B.P. 88° C. Sp.Gr. 0.98.
25% soluble in water, miscible with alcohol and oils, soluble in *Propylene* glycol and Glycerin.

Very powerful and diffusive, pungent, buttery odor. Chlorine-Quinone-like in high concentration, oily-buttery in extreme dilution.

This ketone is very common in Nature, although usually in trace amounts only: in essential oils, flower absolutes, dairy products, meat and fruits, etc.

It finds some use in perfumery – mainly in the re-construction of essential oils (artificial essential oils and flower absolutes). Lavender, Lavandin, Bay, Orris and many other oils contain traces of this ketone.

Finds extensive use in flavor compositions, primarily in imitation Butter, Milk, Cream, Cheese, etc. Also in Berry flavors, Butterscotch, Caramel, Chocolate, Coffee, Cherry, Fruit, Honey, Liquor, Tobacco, Rum, Wine, Nut, Almond, Spice, Ginger Ale, Cream Soda, Vinegar, Vanilla, Buttermilk, etc.

Normal concentration in consumer product will be about 3 to 30 ppm, while it may be as high as 40 to 50 ppm in baked goods. Imitation Butter may contain about 6 to 9 ppm.

G.R.A.S. F.E.M.A. No.2370.

Prod.:

1) from Methyl ethyl ketone.
2) by selective fermentation of Glucose.

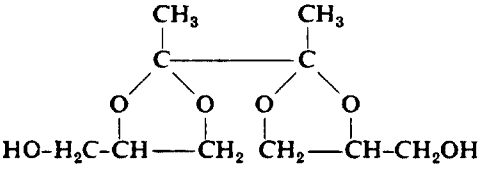
1-261; 4-41; 26-474; 77-210; 85-56; 86-42; 100-332; B-I-769;

NOTE: Fire hazard – flash point is below room temperature.

## 873: DIACETYL GLYCEROL

Diacetylglycerin.

An addition-product of Diacetyl and Glycerin.



$C_{10}H_{18}O_6 = 234.25$

Very viscous, pale yellowish liquid.

Soluble in water, miscible with alcohol and Propylene glycol, soluble in most flavor materials, but not in all Citrus oils.

This peculiar material, although basically consisting of above chemical, is a rather ill-defined chemical as it comes when commercially available. It is occasionally prepared by the user himself, but it has also been available from various European suppliers.

The product is intended for use in flavor compositions, where a milder Diacetyl-effect is desirable, and greater stability necessary. Diacetyl is a very reactive Ketone, and it will form products with many common flavor materials, thereby causing a change in flavor, color and appearance of the finished flavor.

The taste of this material is basically the same as that of Diacetyl, but it is much weaker, a fact which is often translated as "milder", but it will, eventually, release the amount of Diacetyl originally used in making the said amount of adduct.

With proper use of Diacetyl, often in combination with Acetyl methyl carbinol, it is rarely necessary to use such addition products.

Prod.: from 2 Mol. Glycerin plus 1 Mol. Diacetyl by condensation and removal of 2 Mol. water.

4-42;

## 874: DIALLYL DISULFIDE

Allyl disulfide.

$(CH_2{=}CH{-}CH_2)_2S_2$

$C_6H_{10}S_2 = 146.28$

Colorless or pale yellowish mobile liquid.

Very slightly soluble in water, soluble in alcohol, miscible with oils. Sp.Gr. 1.02. B.P. 198 (under slight decomposition).

Pungent odor, not truly reminiscent of Garlic, but heavier, more "sulfide-like", obnoxious odor.

Taste – only in extreme dilutions resembling that of Garlic.

Used in flavor compositions, mainly for imitation Garlic, Onion, Spice-blends, etc.

Concentration in the finished product is about 5 to 8 ppm.

G.R.A.S. F.E.M.A. No.2028.

Prod.:

1) From Allyl bromide plus Sodium thiosulfate to produce Sodium allyl thiosulfate, which is heated and produces Diallyl disulfide.
2) From Allyl mercaptan and Iodine.

50-301; 66-349; 90-828; see also: Diallyl sulfide;

## 875: DIALLYL ETHER

Allyl ether.

$(CH_2{=}CH{-}CH_2)_2O$

$C_6H_{10}O = 98.14$

Colorless mobile liquid. B.P. 94° C.
Sp.Gr. 0.83.

0.3% soluble in water, miscible with alcohol and oils.

Pungent odor, reminiscent of Radish.

Suggested for use in flavor compositions for meat, vegetable juices, condiments, etc.

NOT approved for food in the U.S.A.

Prod.: by dehydration of Allyl alcohol.

26-394; 100-36; B-I-438;

## 876: DIALLYL SULFIDE

Allyl sulfide.
2-Propenyl sulfide.
Thioallyl ether.
NOTE: Do NOT confuse this with Diallyl disulfide (see that monograph).

$(CH_2{=}CH{-}CH_2)_2S$

$C_6H_{10}S = 114.21$

Colorless mobile liquid. B.P. 139° C.
Sp.Gr. 0.89.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, penetrating Garlic-Radish-like odor of poor tenacity. Not a lachrymator, but does produce some irritation of eyes and mucous membranes.

Sweet, Radish-Garlic-like taste in extreme dilution. Greener and sharper odor and taste when compared to Diallyl disulfide.

This material finds use in meat and soup flavors to support the effect of Garlic oil, and to "sharpen" the odor of the Garlic. It is also used in Garlic powders and various condiment blends.

Traces are occasionally used in imitation fruit flavors for powerful topnote effect and "lift".

Concentration is usually 20 to 50 ppm in soup and meat products, or about 1 to 5 ppm as an additive in fruit flavors, calculated upon the finished product.

G.R.A.S. F.E.M.A. No.2042.

Prod.: from Allyl iodide plus Potassium sulfide in alcohol.

26-474; 66-348; 90-828; 100-38; 160-794; B-I-440;

## 877: DIAMYLKETONE

Amylketone.
Di-*n*-amylketone.
Caprone.
Undecan-6-one.

$C_5H_{11}{-}CO{-}C_5H_{11}$

$C_{11}H_{22}O = 170.30$

Leafy crystals or pale yellowish liquid.
M.P. 15° C. B.P. 228° C. Sp.Gr. 0.83.

Insoluble in water, soluble in alcohol and oils.

Ethereal, but not winey, rather solvent-like, unnatural odor with sweet undertone of remotely fruity character.

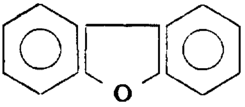
Has been suggested for use in perfume compositions, but does not seem to offer any interesting effects, not even in masking odors for industrial purposes.

Prod.: from Caprone dicarboxylic acid with dilute sulfuric acid.

26-478; 66-517; B-I-714;
(see also No. 189)

## 878: DIBENZOFURAN

Biphenylene oxide.
Diphenylene oxide.



Colorless leaflets. M.P. 85° C. B.P. 287° C.

Practically insoluble in water, somewhat soluble in alcohol, soluble in oils.

Powerful and diffusive odor with peculiar dry-floral, almost tarry-medicinal odor in high concentration, pleasant floral and almost sweet in extreme dilution.

This chemical has been suggested for use in place of Indole with a more pronounced Narcissus effect, and with good possibilities in Oakmoss products. It lends a natural dry note to moss, and introduces power in Lily and Narcissus bases.

Unlike most Furans, this chemical is stable in alkali.

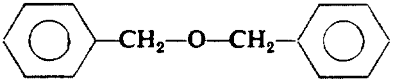
Prod.:

1) from coal tar.
2) from Phenol or Diphenylether by heating with lead oxide.
3) by dehydration of *2,2*-Dihydroxy diphenyl.

1-768; 4-23; 69-192; 5-350;

## 879: DIBENZYLETHER

Benzylether.
Benzyl oxide.



$C_{14}H_{14}O = 198.27$

Colorless oily liquid. M.P. 3° C.
B.P. 297° C. Sp.Gr. 1.03.

Insoluble in water, soluble in alcohol, miscible with oils.

Faint, sweet odor of Anisaldehyde character, but much weaker. Certain commercial lots have "Almond" odor, but the author believes this may be decomposition product (Benzaldehyde). Dibenzylether decomposes slowly in aqueous media to Benzaldehyde.

It finds some use in perfume compositions, particularly in low cost floral fragrances for soap, where its fruity-floral sweetness performs well for Rose, Lilac, etc.

This ether found some use as a solvent for crystalline perfume materials, Nitromusks, etc. but is no longer used or this purpose.

Finds use in flavor compositions, mainly in Fruit, Spice and Nut compounds. Its instability in aqueous media is a disadvantage.

Concentration is normally about 25 ppm in candy or baked goods, while it can be 150-175 ppm in chewing gum.

Prod.:

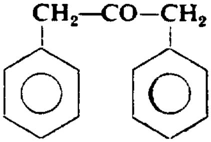
1) by heating Benzylalcohol with dilute sulfuric acid.
2) by heating Benzyl chloride with aqueous alkali.

G.R.A.S. F.E.M.A. No.2371.

4-21; 5-224; 26-430; 31-145; 68-502; 86-43; 100-139; 103-278; B-VI-434;

## 880: DIBENZYL KETONE

Benzyl ketone.
*1,3*-Diphenyl-*2*-propanone.
*alpha-alpha'*-Diphenylacetone.



$C_{15}H_{14}O = 210.28$

White crystals or colorless crystalline mass. M.P. 40° C. B.P. 331° C.

Almost insoluble in water, soluble in alcohol and oils, poorly in Propylene glycol.

Sweet, but rather faint, fruity-almondy odor of considerable tenacity.

Occasionally used as a trace ingredient in floral perfume compositions, Fougère types, New Mown Hay, etc. where it can act as a modifier for Coumarin, making its odor softer.

Used in fruit flavor compositions, and in imitation Honey, Nut, etc. – mostly in traces only.

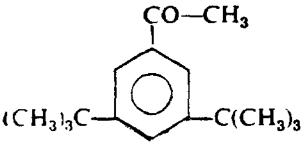
Prod.: by Friedel-Craft's synthesis from Toluene and Phenylacetylchloride (in presence of Aluminium chloride).

G.R.A.S. F.E.M.A. No.2397.

26-480; 36-1257; 68-1169; B-VII-445;

## **881:** 3,5-**DI**-tertiary-**BUTYLACETOPHENONE**

*1*-Acetyl-*3,5*-di-*tertiary*-butyl benzene.



$C_{16}H_{24}O = 232.37$

Colorless liquid, solidifying in the cold to an opaque crystalline mass.

Insoluble in water, soluble in alcohol and oils.

Sweet, floral-animal, musky type of odor with good tenacity. Harsher and less tenacious than Musk Ambrette and Musk Ketone, but has an overall resemblance to the Nitromusks.

This ketonic musk was developed when it became evident that a great number of di-alkyl substituted Acetylbenzenes had interesting odors, often in the musky or Ambre-like type. The *tertiary*-Butyl radicle is often involved in musk odors, and the Acetyl group has successfully been replaced with an aldehyde group, producing further, interesting odorants.

Although patented (1956), this material has had very little success and is probably not commonly used in perfumery. The development of new synthetic musks took such an enormous speed during the late 1950's and early 1960's, that a good number of highly interesting, reasonably inexpensive and very effective musks were commercially marketed.

163-340;

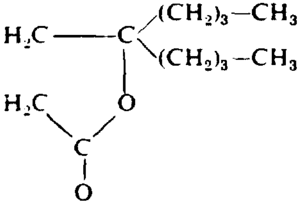
## **882:** 4,4-**DIBUTYL**-gamma-**BUTYROLACTONE**

Dibutyl butyrolactone.

"Dodecanolide" (incorrect name).

*4*-Butyl-*4*-hydroxyoctanoic acid, *gamma*-lactone.

*4,4*-Dibutyl-*4*-hydroxybutyric acid, *gamma*-lactone.



$C_{12}H_{22}O_2 = 198.31$

Almost colorless oily liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Oily, Coconut-buttery odor of considerable tenacity. In suitable dilution (best about 5 ppm in sweetened milk) it displays a pleasant creamy-Coconut-like taste.

Very rarely used in perfume compositions.

Used quite frequently in flavor compositions, mainly for imitation Butter, Coconut, Nut, etc.

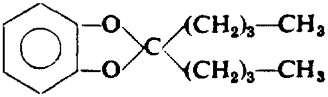
Concentration in the finished consumer product is normally about 3 to 15 ppm. Ice cream demands a somewhat higher level as compared to candy.

Prod.: (many methods): e. g.: from Butyl pentanol and Methylacrylate with a catalyst (Russian patent).

G.R.A.S. F.E.M.A. No.2378.

## 883: DIBUTYL CATECHOL KETAL

Pyrocatechin dibutyl ketal.



$C_{15}H_{22}O_2 = 234.34$

Although not a commercially available item, this chemical has been suggested for use in perfume compositions.

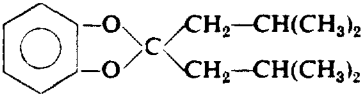
It is described as having a Geranium-Rose type odor.

Prod.: by condensation of Di-*n*-butylketone with Catechol.

31-117;

## 884: DI-iso-BUTYL CATECHOL KETAL

Pyrocatechin di-*iso*-butyl ketal.
Catechol-di-*iso*-butyl ketal.



$C_{15}H_{22}O_2 = 234.34$

Has been suggested for use in perfume compositions. This chemical is a member of a rather large family of ketals, prepared from Di-phenols, Phenol-Alcohols, etc. but very few of these research chemicals have become sufficient popular that a commercial production could be undertaken.

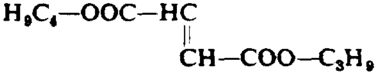
The above chemical is described as having a Geranium-Rose type odor with a Honeylike note.

Prod.: by condensation of Catechol with Di-*iso*-butylketone.

30-253; 31-117; 31-118;

## 885: DIBUTYL FUMARATE

Dibutyl-*trans*-butene dioate.



$$\begin{array}{l} H_9C_4\text{—OOC—HC} \\ \qquad\qquad\qquad\quad \| \\ \qquad\qquad\qquad\quad \text{CH—COO—}C_3H_9 \end{array}$$

$C_{12}H_{20}O_4 = 228.29$

Colorless oily liquid.

Slightly soluble in water, soluble in alcohol and oils.

Sweet-herbaceous, warm and fungoid, but pleasant odor of moderate tenacity.

The title ester has been suggested for use in perfumes, but the author is not aware of its use in flavors, although its aroma type could indicate potential use in certain types of imitation flavor (Mushroom).

The ester gives interesting effects in Lavender compositions, blends well with Oakmoss and Amylsalicylate, and in general with warm-herbaceous notes. It is very mild and generally considered too weak for use in perfumery, where, occasionally, the Allyl ester has found some application.

Prod.: by direct esterification of *n*-Butanol with Fumaric acid.

## 886: DIBUTYL KETONE

Nonanone-*5*.
Valerone.

$(C_4H_9)_2CO$

$C_9H_{18}O = 142.24$

Colorless liquid. B.P. 188° C. Sp.Gr. 0.82.

Insoluble in water, soluble in alcohol and oils.

Oily fruity, somewhat harsh odor with some resemblance to Banana and Passionfruit.

Could find use in masking odors for industrial purposes, but is not commonly used in perfume compositions.

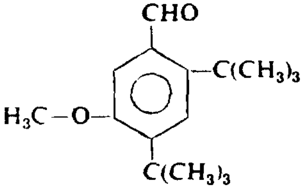
Has been suggested for flavor compositions, mainly as a modifier in various fruit flavor imitations.

Prod.: from Valerone dicarboxylic acid with dilute sulfuric acid.

26-486; 36-1143; 66-517; B-I-709;

## 887: 2,4-DI-tertiary-BUTYL-5-METHOXY BENZALDEHYDE

"Ambral" (Givaudan Corp.).



$C_{16}H_{24}O_2 = 248.37$

Colorless or white crystalline powder.
M.P. 65° C.

Practically insoluble in water, slightly soluble in cold alcohol, soluble in warm alcohol and oils.

This material is today more a milestone in perfume chemistry than it is a perfume material as such. It represents the door through which the perfume chemist came into a world of entirely new musk-smelling chemicals, materials containing no Nitrogen. The title material was produced as an intermediate in the making of new Nitromusks, but it was found to possess a pleasant Ambre-musky type of odor itself – so pronounced, that it became an interesting perfume material until the new Nitrogen-free musks, and many Ambregris-smelling chemicals were developed.

Although only two decades old (Carpenter 1948) this musk has now lost most of its importance af a perfume material. It has a very pleasant and distinctly musky odor, but cannot compete in richness with the newer materials.

Prod.: by oxidation of *2,4*-Di-*tertiary*-butyl-*5*-methoxytoluene.

(Carpenter, U.S. pat. 2,450,879 of Oct. 12, 1948).

The *6*-Methoxy-derivative is known, and it has also a musky odor.

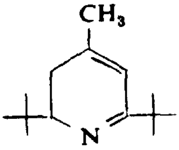
See also:
Di-*iso*-propylbenzaldehyde,
Di-*iso*-propyl dimethylbenzaldehyde.
Di-*iso*-propyl methylbenzaldehyde.
Di-*iso*-propyl phenylacetaldehyde.

The Tri-*iso*-propylbenzaldehyde is also known to possess a musky odor.

163-195;
(see also "Givaudanian", Febr. 1968).

## 888: DI-iso-BUTYL-gamma-PICOLINE

*2,6*-Di-*iso*-butyl-*4*-methylpyridine.



$C_{14}H_{23}N = 205.35$

Colorless or pale straw-colored oily liquid.

Slightly soluble in water, soluble in alcohol and oils.

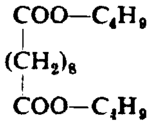
Sweet Oakmoss-like penetrating odor with floral undertones. The odor quality of this product is very strongly dependent upon the purity of the chemical. This is typical of many Pyridine derivatives, in which traces of unreacted Pyridine or other impurities may completely ruin the true and often very pleasant picture of the odor of the derivative.

The title material finds a little use in perfume compositions, often in conjunction with Oakmoss products, or in the sweeter types of "Leather" fragrance. It blends very well with Amylsalicylate, the Phenylacetates, Ionones, Hydroquinone dimethylether, etc.

Prod.: from *2,4*-Dimethylpyridine and Benzaldehyde, followed by treatment of the Pyridine hydrochloride with *iso*-Butylchloride in the presence of a Copper catalyst.

## 889: DIBUTYL SEBACATE

Dibutyl decanedioate.
*n*-Butyl sebacate.



$$\begin{array}{l} COO{-}C_4H_9 \\ | \\ (CH_2)_8 \\ | \\ COO{-}C_4H_9 \end{array}$$

$C_{18}H_{34}O_4 = 314.47$

Colorless oily liquid. Sp.Gr. 0.93.
B.P. 345° C.

Insoluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol.

Fruity, but very mild and oily odor of considerable tenacity. To some people it appears virtually odorless.

Very faint, fruity-oily taste.

Finds little or no use in perfume compositions, except ocasionally as a solvent for Oakmoss concrete.

Used in flavor compositions, mainly in imitation fruit flavors, normally in traces only. It seems to introduce a certain mildness and to round the harsher notes from more volatile flavor chemicals. The effect is particularly noticeable in Banana and other mild, non-juicy flavor types.

Prod.: by direct esterification of *n*-Butanol with Sebacic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2373.

4-26; 26-486; B-II-719;

## 890: DIBUTYL SULFIDE

*n*-Butylsulfide.

$(C_4H_9)_2S$

$C_8H_{18}S = 146.30$

Colorless liquid. Sp.Gr. 0.84. B.P. 182° C.

Insoluble in water, soluble in alcohol and oils.

Very powerful, repulsively sulfuraceous odor in high concentration. Intensely green, foliage-odor in extreme dilution. Solutions weaker than 5% in Diethyl phthalate show little or no "sulfide"-type odor, and the green odor is typical and perceptible at far below 0.2% in the same solvent.

Very useful as a natural green topnote in Geranium and Violet bases. Its effect has been compared to that of Methyl heptin carbonate, but it is actually cleaner, absolutely non-fatty and easier to apply to a compound than the MHC. There is less chance of over- and under-dosage with the sulfide.

Used in flavor compositions, not only in the rare type of Violet, but also in various florals and fruit flavor types. The concentration in the finished product amounts to mere traces.

G.R.A.S. F.E.M.A. No.2215.

Prod.: from Dibutyl bromide plus Potassium sulfide.

26-486; 66-348; B-I-370;

## 891: DI-n-BUTYRYL

4,5-Octanedione.
Dipropyl diketone.

$CH_3(CH_2)_2—CO—CO—(CH_2)_2CH_3$

$C_8H_{14}O_2 = 142.20$

B.P. 168° C.  Sp.Gr. 0.93.

Intensely yellow liquid. Slightly soluble in water, miscible with alcohol and oils. Soluble in Propylene glycol and Glycerin (but develops additive products with these).

Powerful and pungent, fatty-buttery odor in high concentration. Pleasant creamy-buttery and rather sweet in extreme dilution.

Oily-sweet, buttery taste, often with a slightly cheesy note.

This chemical is used in flavor compositions, mainly for imitation Butter, Cream, Cheese, Milk, etc. and also in Rum, Butterscotch and various flavor compositions for baked goods, candy, etc.

NOT listed as G.R.A.S. in the Federal Register of the U.S.A.

Prod.: by oxidation of Butyroin (Butyryl propyl carbinol).

4-43; 66-721; 86-43;

## 892: DI-iso-BUTYRYL

Di-*iso*-propyl diketone.

$(CH_3)_2CH—CO—CO—CH(CH_3)_2$

$C_8H_{14}O_2 = 142.20$

Intensely yellow, oily liquid.  Sp.Gr. 0.92.
B.P. 145° C.

Slightly soluble in water, miscible with alcohol and oils. Soluble in Propylene glycol and Glycerin.

Sharp and pungent, fruity-buttery odor, sharper, fruitier and sweeter than that of the Di-*n*-butyryl, not as cheese-like. Oily buttery, somewhat sweet-fruity taste in high dilution. Has been suggested for use in flavor compositions, but it seems to lend a sharper, harsher, less natural note than what can be obtained with the Di-*n*-butyryl.

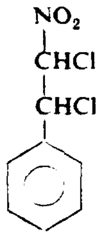
NOT listed as G.R.A.S. in the U.S. Federal Register.

Prod.: by oxidation of *iso*-Butyroin (*iso*-Butyryl-*iso*-propyl carbinol).

66-721; 86-46;

## 893: DICHLOROPHENYL NITROETHYLENE

Phenyl dichloro nitroethylene.



$C_8H_7Cl_2NO_2 = 220.07$

Yellowish oily liquid, or yellowish needle-like crystals, melting at 30° C.

Practically insoluble in water, soluble in alcohol, miscible in oils.

Extremely powerful, diffusive, gassy-fruity odor. In very high dilution pleasantly Apple-like with a rose-like sweetness.

In aqueous dilution below 10 ppm, the flavor is sweet, ethereal, intensely Apple-like with a rosy undertone.

This peculiar chemical is mentioned partly because of its unusual power and fragrance type, partly because it is one of the oldest of all "unconventional" fragrance materials. It dates back before the turn of the Century, probably about 1892.

The European Apple, Reinette, is a favorite cooking Apple, and its aroma is surprisingly well duplicated by the subject chemical. The author has his doubts that such a chemical would be found in a fruit, and it is most conceivable that the material carries a certain hazard, judging from its structure and composition, to the human health.

Prod.: by chlorination (bubbling Chlorine) of Phenyl nitroethylene in dry Chloroform solution.

72-7;

## 894: DICROTYL SULFIDE

2-Butenyl sulfide. (*cis*- and *trans*- are known).

$(CH_3{-}CH{=}CH{-}CH_2)_2S$

$C_8H_{14}S = 142.27$

Pale yellowish liquid. B.P. 185° C.

Penetrating and repulsive "Skunk" odor.

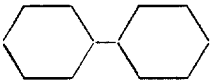
Has been suggested for use in artificial Civet bases, but the author finds that this odor type is not the desirable one in the Civet odor complex. Although it cannot be classified as "fecal", the odor of this Sulfide is unpleasant at practically any level down to the minimum perceptible.

Prod.: from Crotyl bromide and Potassium sulfide.

86-43; 65-731;

## 895: DICYCLOHEXYL

Dodecahydrodiphenyl.



$C_{12}H_{22} = 166.31$

Colorless liquid. Solidifies in the cold, melts at 3° C. B.P. 214° C. Sp.Gr. 0.89.

Insoluble in water, soluble in alcohol and oils.

Sweet, mild-aromatic, but rather "chemical" odor.

Has been suggested for use in perfume compositions, mainly as a modifier in low-cost Geranium, New Mown Hay, Lavender, Rose and other bases.

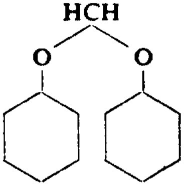
It imparts a certain "lift" to the composition, enough to make it interesting in soap and detergent perfumes, but there are chemicals that lend a much better effect of this type at lower cost.

Prod.: (several methods) e. g.: by catalytic reduction of Diphenyl.

4-43; 67-294; 86-43;

## 896: DICYCLOHEXYL FORMAL

Formaldehyde dicyclohexylacetal.
Dicyclohexyl methylal.



$C_{13}H_{24}O_2 = 212.34$

Colorless liquid.

Slightly soluble in water, soluble in alcohol and oils.

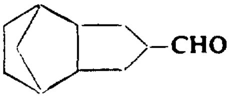
Sweet ethereal odor of moderate to poor tenacity. Its fruity notes are pleasant, but not characteristic of any particular fruit. This acetal has been suggested for use in perfume compositions, but it does not seem to have attracted much interest. It lacks character and does not lend any unusual notes or effects not obtainable with other perfume chemicals.

Prod.: by condensation of Formaldehyde with Cyclohexanol. The material may also be prepared from Cyclohexanol and Methyl-*ortho*-formate.

## 897: DICYCLOPENTADIENE ALDEHYDE

Exo-*3A*,-*4*,*5*,*6*,*7*,*7A*-hexahydro-*4*,*7*-methanoindane-*2*-carboxaldehyde.

(exo-isomer):



$C_{11}H_{16}O = 164.25$

Colorless viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

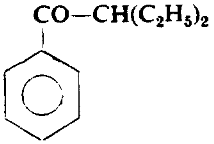
Very powerful and diffusive, fresh, vegetable-green odor, sometimes classified as "Ozone-like" or Melon-like. Its odor has also been compared to that of fresh sap from wood or bark.

Has found some use in perfumery, mainly as a modifier in green odor bases, topnotes, etc. and to impart freshness to woody fragrances.

Prod.: from Dihydro dicyclopentadiene.

## 898: omega-omega-DIETHYL ACETOPHENONE

*1*-Phenyl-*2*-ethylbutan-*1*-one.



$C_{12}H_{16}O = 176.26$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Sweet and rather mild Bitter-Almond type odor with herbaceous-haylike undertone.

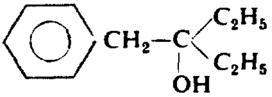
This ketone, rarely offered under its proper name, occasionally used in perfume specialties, finds a little use as a sweetener of good tenacity in herbaceous or herbaceous-woody-floral fragrance types, e. g. Lilac, Lavender, Mimosa, Fougère, Chypre, etc.

Prod.: e. g. from Phenyl-*2*-ethylbutylcarbinol by oxidation.

3-182;

## 899: DIETHYL BENZYL CARBINOL

*alpha*-Benzyl-*secondary*-amylalcohol.
Benzyl diethyl carbinol.
*beta*-Hydroxy-*beta*-benzylpentane.



$C_{12}H_{18}O = 178.28$

Colorless oily liquid. Sp.Gr. 0.97.
B.P. 248° C.

Green-floral, slightly oily and rather heavy-odor of good tenacity.

A comparatively rare commercial item. Has never been able to substitute or compete with the Dimethyl benzyl carbinol.

Finds a little use in perfume compositions, mainly in the green-floral types.

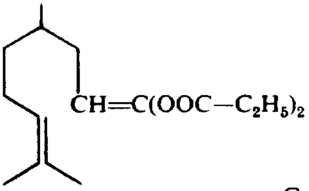
Prod.: from Diethyl acetone and Benzyl magnesium bromide.

4-42;

## 900: DIETHYLCITRONELLIDENE MALONATE

Citronellidene diethylmalonate. (?)

1)



$C_{17}H_{28}O_4 = 296.41$

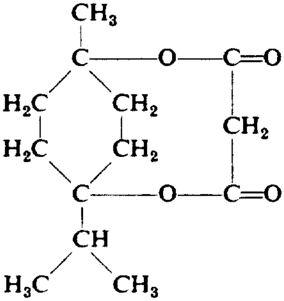
Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

This relatively rare chemical, occasionally available under trade name, finds limited use in perfume compositions. There has been considerable doubt about the actual structure of a material under this name.

The aldehyde Citronellal will form a condensation product with Malonic acid. The condensation product may eventually become a Lactone of the theoretical structure:

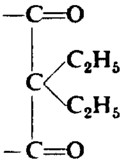
(2)



or:

$C_{13}H_{20}O_4 = 240.30$

(3)



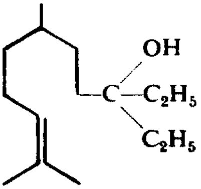
$(C_{17}H_{28}O_4 = 296.41)$

While a condensation with Diethylmalonate is theoretically possible, the author is inclined to believe that the material mentioned in literature (and possibly misnamed) could be the Lactone-form (structure No.3). In any event, this chemical is included in the present work in order to describe one rare group of chemicals of possible interest to the perfumer.

If Diethylmalonic acid is used, the alternative (3) may occur. That material could bear the name Diethylcitronellidene malonate.

## 901: DIETHYL CITRONELLOL

1,1-Diethylcitronellol.
(Commercial products contain also Diethyl geraniol).



$C_{14}H_{28}O = 212.38$

Almost colorless liquid. Insoluble in water, soluble in alcohol and oils.

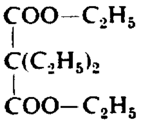
Camphoraceous-rosy, rather faint odor, overall more crude and harsh than that of Citronellol.

Not a very interesting perfume material.

30-406; 31-17; 159-607;

## 902: DIETHYL DIETHYLMALONATE

"Diethyl malonic ester".



$$\begin{array}{l} COO-C_2H_5 \\ | \\ C(C_2H_5)_2 \\ | \\ COO-C_2H_5 \end{array}$$

$C_{11}H_{20}O_4 = 216.28$

Colorless oily liquid. B.P. 230° C.

Almost insoluble in water, soluble in alcohol and oils.

Quite powerful, fruity, Pear-like odor.

The author cannot agree with odor descriptions that include the words "Cumin", "Anise", etc. and he believes this must refer to a different chemical.

This ester has been suggested for use in flavor compositions but it is not sufficiently stable that it can become very popular.

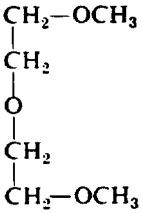
The ester has occasionally found use in perfume compositions, mainly as a modifier in fruity notes, winey topnote bases, etc.

Prod.: (several methods) e. g. by condensing Ethyl acetate with Ethyl oxalate, heat the resultant Oxaloacetic ester, and esterify the formed Diethyl malonic acid.

4-42; 31-170; 66-968;

## 903: DIETHYLENEGLYCOL DIMETHYLETHER

Methyl Carbitol.
Dimethyl carbitol.
"Diglyme".
(see also: Diethyleneglycol monomethylether).



$$\begin{array}{l} CH_2-OCH_3 \\ | \\ CH_2 \\ | \\ O \\ | \\ CH_2 \\ | \\ CH_2-OCH_3 \end{array}$$

$C_6H_{14}O_3 = 134.18$

Colorless, slightly viscous liquid.

Sp.Gr. 0.95. B.P. 161° C.

Miscible with water and alcohols. Soluble in most oils, poorly in mineral oil and many other hydrocarbons.

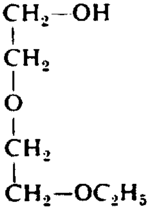
This chemical serves mostly as a solvent for perfume materials, but it is not quite odorless and therefore not as desirable as Diethylphthalate. However, the fact that it is miscible with aqueous phases makes it useful in certain cases, where Diethyl phthalate would be useless.

NOT to be used in flavors (comparatively toxic).

66-667; 100-359;

## 904: DIETHYLENEGLYCOL MONOETHYLETHER

Ethyl Diethylene glycol.
"Carbitol".
Enkanol.



$$\begin{array}{l} CH_2-OH \\ | \\ CH_2 \\ | \\ O \\ | \\ CH_2 \\ | \\ CH_2-OC_2H_5 \end{array}$$

$C_6H_{14}O_3 = 134.18$

Colorless hygroscopic liquid. Miscible with water, alcohol and most oils. Sp.Gr. 0.99. B.P. 202° C.

Faint, ethereal odor with a musty undertone.

Bitter taste is perceptible at concentrations above 20 ppm.

This chemical is used mainly as a solvent for perfume materials, NOT suitable for flavors.

It is considered more toxic than Ethylene glycol, and therefore banned from food flavors in most countries.

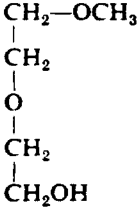
As a solvent for perfume materials it is of very limited value, since it has a significant vapor pressure, enough to "lift" certain odors, yet at the same time it cannot be classified as volatile. It is not highboiling enough to be used as a fixative, not low-boiling enough to be used in place of alcohol.

Prod.: (several methods) e. g.: as a by-product in the manufacture of Cellosolve (Ethylene glycol monoethylether) from Ethyl alcohol plus Ethylene oxide.

26-450; 66-667; 100-209; B-I-520, Zweiter Ergzbd.;

## 905: DIETHYLENEGLYCOL MONOMETHYLETHER

"Methyl Carbitol".
(Sometimes called "Carbitol" commercially).
(see also: Diethyleneglycoldimethylether).



$$\begin{array}{l} CH_2\text{—}OCH_3 \\ | \\ CH_2 \\ | \\ O \\ | \\ CH_2 \\ | \\ CH_2OH \end{array}$$

$C_5H_{12}O_3 = 120.15$

Colorless liquid. B.P. 193° C. Sp.Gr. 1.04.

Miscible with water, alcohol and most oils. Not clearly soluble in mineral oil and many Terpenes, other hydrocarbons, etc.

Faint, rather dry-musty, somewhat ethereal odor, not exactly pleasant.

The odor seems to vary considerably in lots from different manufacturers. Commercial grade of this chemical is presumably not very pure.

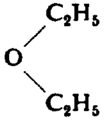
Finds some use as a solvent in perfumes, but has little advantage other than its solubility in water and perfume oils at the same time. It is not volatile enough to substitute alcohol, and not high-boiling enough to act as a fixative-blender.

Occurs as a by-product in the manufacture of Methyl cellosolve.

26-602; 66-667; 100-673;

## 906: DIETHYL ETHER

Ethyl ether.
"Ether".
Ethyl oxide.
Ethoxy ethane.
Sulfuric ether.



$C_4H_{10}O = 74.12$

Colorless, very mobile liquid. B.P. 35° C. Sp.Gr. 0.71.

8 % soluble in water, miscible with alcohol and oils. 1.2 % water is soluble in Ether.

Very diffusive, sweet-ethereal odor. Actually a poor odorant, it gives impression of power by its very high vapor pressure at room temperature.

NOTE: Flammable and highly explosive. Concentrations higher than 55 grams of ether per cubic meter of air present hazard of explosion. (about 1.5 grams of ether per cubic foot of air).

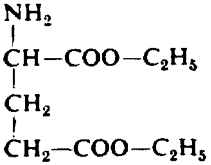
Finds very little, if any, use in perfumes or flavors. However, being a useful extraction solvent for natural perfume and flavor materials, it is often found in traces in the commercial, evaporated extracts. It is easier to remove ether from natural extracts, than it is to remove Hexane and other, more common solvents for perfume raw materials.

Prod.:
1) by dehydration of Ethyl alcohol (with sulfuric acid).
2) by hydration of Ethylene.

26-538; 31-144; 66-323; 100-430; B-I-430;

## 907: DIETHYL GLUTAMATE

Diethyl-*alpha*-glutamate.
*L-alpha*-Glutamic acid, diethylester.



$$\begin{array}{l} NH_2 \\ | \\ CH-COO-C_2H_5 \\ | \\ CH_2 \\ | \\ CH_2-COO-C_2H_5 \end{array}$$

$C_9H_{17}NO_4 = 203.24$

Viscous liquid. B.P. 239° C.

Very soluble in water, soluble in alcohol and most perfume oils.

Very faint, winey-ethereal odor.

In high concentration somewhat bitter taste, in weaker solutions rather sweet, bland, nondescript taste.

Has been attributed synergistic effect upon fragrance mixtures (perfume compositions, etc.).

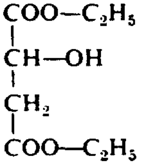
A French patent covers its use as a fragrance-enhancing additive, but experiments seem to confirm that the material is not a universal synergist. Private experiments by the author have not been successful in proving any perceptible effect of the little material.

Prod.: from *L-alpha*-Glutamic acid, by esterification.

86-10; 86-42; 66-1117;
see also: 100-487 and 66-1116;

## 908: DIETHYL MALATE

*dl*-Ethyl malate.
Diethyl hydroxysuccinate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ CH-OH \\ | \\ CH_2 \\ | \\ COO-C_2H_5 \end{array}$$

$C_8H_{14}O_5 = 190.20$

Colorless liquid. Sp.Gr. 1.12. B.P. 254° C.

Soluble in water, miscible with alcohol and oils.

Mild, winey-fruity odor with a pleasant oily-herbaceous undertone, overall reminiscent of the odor of Apple skins (peel).

Mild, fruity-winey taste.

Rarely, if ever, used in perfumery.

Quite frequently used in flavor compositions, mainly for imitation Apple and Rum. The concentration in the finished consumer product may be about 20 to 25 ppm, or up to 45 ppm in baked goods.

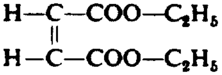
G.R.A.S. F.E.M.A. No.2374.

Prod.: from *dl*-Malic acid plus Ethyl alcohol, using Hydrochloric gas as a condensing agent.

26-500; 66-1105; 158-186; B-III-437;

## 909: DIETHYL MALEATE

Ethyl maleate.
Ethylene-*cis*-dicarboxylic acid*, diethylester.
*(Fumaric acid is the *trans*-isomer).



$$\begin{array}{l} H-C-COO-C_2H_5 \\ \quad \| \\ H-C-COO-C_2H_5 \end{array}$$

$C_8H_{12}O_4 = 172.18$

Colorless liquid. Sp.Gr. 1.07. B.P. 223° C.

Insoluble in water, soluble in alcohol and oils.

Presumably not used in perfume compositions.

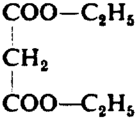
Finds some use in flavor compositions, but its weak and uncharacteristic flavor makes it inferior to the Malonate and Malate. Its use is limited to application in imitation fruit flavors, mainly those for soft drinks and hard candy.

Prod.: by direct esterification of Maleic acid with Ethylalcohol.

26-500; 66-990; 100-432; B-II-751;

## 910: DIETHYL MALONATE

Ethyl malonate.
Malonic ester.
Ethyl propane dioate.
Ethyl methanedicarboxylate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ CH_2 \\ | \\ COO-C_2H_5 \end{array}$$

$C_7H_{12}O_4 = 160.17$

Colorless liquid. Sp.Gr. 1.06. B.P. 199° C.

2% soluble in water, miscible with alcohol and oils.

Sweet, soft and pleasant fruity-green, slightly balsamic odor, reminiscent of Apples.

Mild fruity, sweet taste at 10 to 40 ppm in slightly acidified sugarwater.

Presumably not used in perfume compositions, except in rare cases of fruity-winey topnote compositions, etc.

Finds extensive use in flavor compositions for imitation Apple, Apricot, Berry, Fruit, Grape, Peach, Pear, etc.

Concentration in the finished product will normally be about 20 ppm.

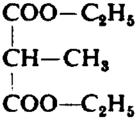
G.R.A.S. F.E.M.A. No.2375.

Prod.: from Cyanoacetic acid and Ethylalcohol with Hydrogen chloride.

4-17; 4-42; 26-500; 31-126; 66-962; 100-432; B-II-573; 160-1084; 8-401; 7-171; 140-147;

## 911: DIETHYL METHYLMALONATE

Methylmalonic acid, diethylester.
(Sometimes called "Methylmalonic ester").



$$\begin{array}{l} COO-C_2H_5 \\ | \\ CH-CH_3 \\ | \\ COO-C_2H_5 \end{array}$$

$C_8H_{14}O_4 = 174.20$

Colorless mobile liquid.

Slightly soluble in water, soluble in alcohol and oils.

Pleasant, light, ethereal odor of good diffusive action and poor tenacity.

This ester is occasionally used in perfumery as part of light topnote-compositions. It may introduce a "mellowness" resembling that of good, well-aged alcohol, an odor type suitable for fragrances intended for use as colognes or diluted perfume lotions.

It performs well with the Citrus oils, Neroli, with green topnotes and winey or winey-floral topnotes. It has also useful effect on tinctures, e. g. Ambregris tincture and Civet tincture.

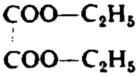
Prod.:

1) by condensing Ethylpropionate with Diethyloxalate, followed by heating of the reaction product.
2) from Diethylmalonate plus Sodium and Methyl iodide.

66-963; 66-966;

## 912: DIETHYL OXALATE

Ethyl oxalate.
Diethyl ethanedioate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ COO-C_2H_5 \end{array}$$

$C_6H_{10}O_4 = 146.15$

Colorless liquid. Very slightly soluble in water (decomposition of the ester), miscible with alcohol and oils.
Sp.Gr. 1.08. B.P. 186° C.

Weak, somewhat musky odor, slightly herbaceous and Mushroom-like.

Very mild taste, in higher concentration somewhat earthy-musty, and slightly burning.

Has been used occasionally as a solvent for perfume materials.

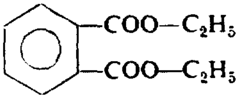
Finds little or no use in flavor compositions, except occasionally in certain gravy and meat flavors, in countries where the use of the ester is permitted.

Prod.: from Oxalic acid and Ethyl alcohol by azeotropic esterification.

26-500; 38-I-609; 31-126; 77-179; 100-354; B-II-535; 140-146;

## 913: DIETHYL PHTHALATE

Diethyl-*ortho*-phthalate.
Ethyl phthalate.
Phtalol.
Neantine (Givaudan).
Solveol.
Anozol. (Fritzsche).
D.E.P.
and many other names and trade names.



$C_{12}H_{14}O_4 = 222.24$

Colorless oily liquid, insoluble in water, soluble in alcohol and oils. Sp.Gr. 1.12.
B.P. 298° C.

Virtually odorless when pure ("Perfumery grade" of commercial Diethyl phthalate).

Very bitter taste in weak hydro-alcoholic solution. Bitter taste perceptible below 20 ppm.

Widely used as a solvent and diluent for powerful or nonpourable perfume materials. Aldehydes, Indole, Skatole, flower absolutes, Resinoids, etc. are often diluted to convenient strength or viscosity with D.E.P.

The older – and by and large abandoned – practise of using D.E.P. as a diluent for perfumes, e. g. for the purpose of adjusting the cost, is a very poor idea, since D.E.P. acts as an odor depressant, not really as a fixative or an innocuous diluent. A 20% solution of a perfume in D.E.P. smells not only weaker than a 20% solution of the same perfume in alcohol, but it smells quite different, due to the physical action of D.E.P. upon the volatile perfume components.

It is generally considered undesirable to use D.E.P. in higher concentration than absolutely necessary for the above first named purposes. There are indications that the solvent at higher concentrations is irritant to a higher than average percentage of human skin, as compared to other perfume ingredients.

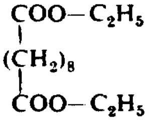
The toxicity of D.E.P. is considered equal to that of Ethylene glycol, or much lower than the toxicity of *Dimethyl* phthalate.

Prod.: by direct esterification of Phthalic acid with Ethyl alcohol. Also from Phthalic anhydride.

4-17; 7-172; 26-500; 63-76; 68-844; 86-19; 34-806; 85-56; 100-434; 106-274; B-IX-798;

## 914: DIETHYL SEBACATE

Ethyl sebacate.
"Sebacyl ether".
Ethyl decane dioate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ (CH_2)_8 \\ | \\ COO-C_2H_5 \end{array}$$

$C_{14}H_{26}O_4 = 258.36$

Colorless oily liquid. Solidifies in the cold, melts at 1.5° C. B.P. 306° C. (decomposition of the ester). Sp.Gr. 0.97.

0.15% soluble in water, soluble in alcohol and oils.

Faint, but pleasant, winey-fruity odor, resembling that of Quince and Melon.

Occasionally used in perfume compositions as a solvent-diluent.

Used in flavor compositions for imitation Apple, Butter, Coconut, Melon, Nut, Peach, Pear, Cherry, Gooseberry, Quince and in many combination flavors.

Concentration in the finished product is normally about 40 ppm (baked goods), while it may come as high as 500 ppm in chewing gum.

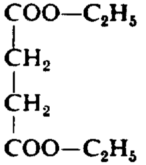
Prod.: by direct esterification of Sebacic acid with Ethyl alcohol, e. g. under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2376.

4-42; 7-173; 26-500; 31-126; 33-821; 66-985; 77-189; 86-42; 95-183; 100-435; B-II-719; 140-147;

## 915: DIETHYL SUCCINATE

Ethyl succinate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ CH_2 \\ | \\ CH_2 \\ | \\ COO-C_2H_5 \end{array}$$

$C_8H_{14}O_4 = 174.20$

Colorless liquid, slightly soluble in water, soluble in alcohol and oils. Sp.Gr. 1.04.
B.P. 218° C.

Faint, pleasant odor, remotely winey-ethereal. The odor type is somewhat similar to that of Ethyl benzoate, but of much less power. Burning taste in high concentration, mildly tart-fruity upon dilution.

Finds some use as a solvent-fixative in perfumery.

Used in various flavor compositions, such as imitation Butter, Rum, Arak, Brandy, Grape, Raspberry, Orange, etc. In Europe, it has found more use in imitation Blackcurrant, a flavor which it is extremely difficult to imitate artificially.

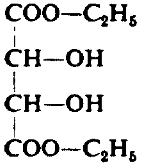
Prod.: by azeotropic esterification or ordinary esterification of Succinic acid and Ethyl alcohol, or Succinic Anhydride and Ethyl-alcohol.

G.R.A.S. F.E.M.A. No.2377.
E.O.A. No.247.

4-42; 7-173; 26-500; 66-970; 77-189; 86-42; 95-183; 96-209; 100-436; 158-186; B-II-609; 140-146;

## 916: DIETHYL TARTRATE

Ethyl tartrate.
Commercial product is *dextro*-tartrate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ CH-OH \\ | \\ CH-OH \\ | \\ COO-C_2H_5 \end{array}$$

$C_8H_{14}O_6 = 206.20$

Colorless viscous liquid. Sp.Gr. 1.20. Solidifies in the cold, melts at 17° C. B.P. 280° C.

Slightly soluble in water, miscible with alcohol and oils.

Very faint, winey odor.

Of little or no use in perfumery.

Finds some use in flavor compositions as a solvent, and since it is often used at fairly high concentration, it does impart some flavor to such compositions. It can be considered as a mild blender for fruity and winey flavor types.

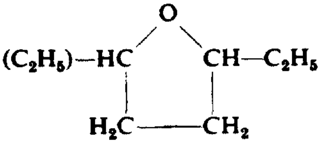
The concentration in finished goods is normally about 200 ppm. (in baked goods, candy, icecream, etc.).

Prod.: by direct esterification of Tartaric acid with alcohol.

G.R.A.S. F.E.M.A. No.2378.

4-18; 4-42; 26-502; 100-436; B-III-512;

## 917: 2,5-DIETHYL TETRAHYDROFURAN



$C_8H_{16}O = 128.22$

Colorless liquid. B.P. (approximately) 116° C.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and diffusive, sweet-herbaceous, caramellic odor of very poor tenacity.

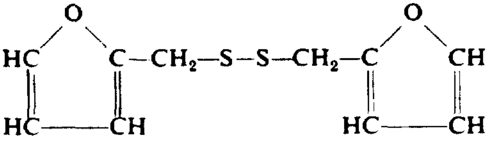
This material has recently become commercially available after many years of hiding in research laboratories or "captive" use by a few manufacturers. It finds use almost exclusively in the reconstruction of certain essential oils, used in flavor compositions, particularly members of the Mint family.

Due to the very high vapor pressure (at room temperature) of this material, it will probably not find any use in perfume compositions, except as a component of certain artificial essential oils or bases, entering the perfume as minor base-components ("subcompounds").

(Sample: The Glidden Company, Organic Chemicals Division).
(See also: 69-166).

## 918: DIFURFURYL DISULFIDE

Furfuryl disulfide.



$C_{10}H_{10}O_2S_2 = 226.32$

Pale yellowish oily liquid.

Slightly soluble in water, soluble in alcohol and oils.

Powerful, repulsively sulfuraceous (sulfide-like) odor, only in extreme dilution becoming attractive, caramellic-burnt, "roasted" odor.

This chemical has been made available recently after its being identified in the volatile oil from roasted Coffee.

It has found use in the flavor bases which are used to re-constitute the aroma of instant Coffee and other Coffee products. It is also used in imitation Coffee flavor.

Another Coffee flavor component, Furfuryl mercaptan, is produced by reduction of the above disulfide.

Prod.: from Furfural and Hydrogen sulfide gas.

69-151;

## 919: DIHEPTYL ETHER

*n*-Heptyl ether.

$C_7H_{15}—O—C_7H_{15}$

$C_{14}H_{30}O = 214.39$

Colorless liquid. Sp.Gr. 0.81. B.P. 262° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar fatty "wet wool" odor, with notes often described as "metallic".

Apart from occasional use in the reconstruction of certain essential oils, etc. (artificial Costus, etc.), this ether is of little or no value to the creative perfumer.

To the author's knowledge, this ether is not used in flavor compositions.

Prod. by dehydration of *n*-Heptanol.

31-144; 26-504; 86-43; B-I-414;

## 920: DI-beta-gamma-HEXENYLETHER

*cis-3*-Hexenylether.

$(CH_3—CH_2—CH{=}CH—CH_2—CH_2)_2O$

$C_{12}H_{22}O = 182.31$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Powerful "gassy"-green, rather choking odor, in high concentration almost cabbage-like, but not sulfuraceous. At proper dilution, the odor has some similarity to the odor of Orange leaf (or Bitter Orange leaf water oil).

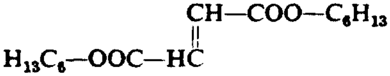
Although a very rare item, this chemical finds some use in perfumery, mainly in the reconstruction of essential oils and flower absolutes.

Prod.: by dehydration of "Leaf alcohol" (*cis-3*-Hexenol).

3-169; 4-190;

## 921: DIHEXYL FUMARATE

Hexyl fumarate.
Dihexyl-*trans*-butene dioate.



$$\begin{array}{r l} & CH—COO—C_6H_{13} \\ & \| \\ H_{13}C_6—OOC—HC & \end{array}$$

$C_{16}H_{28}O_4 = 284.40$

Colorless liquid. Sp.Gr. 1.01. B.P. 278° C.

Almost insoluble in water, soluble in alcohol and oils.

This ester has found use in perfumery for its effect which resembles that of the Tiglic and Angelic esters of Amyl- and Hexyl alcohols. It has warm, herbaceous-winey, slightly green and quite tenacious odor of versatile use in perfumery.

Not confined to the Chamomile type of herbaceous notes, this ester can supply fixation of the herbaceous notes in Lavender, Geranium, Lavandin, Rosemary, Clary sage, etc. and it blends well into Fougères, Chypres, Oriental types, etc.

The title ester has the advantage of being much less expensive than the Tiglic and Angelic esters, and since Fumaric acid is commercially available in high grade of purity, it also offers an ester free from isomers (until recently, Tiglic acid was not available at reasonable cost unless accompanied by a considerable amount of Angelic acid).

Prod.: by direct esterification of *n*-Hexanol with Fumaric acid under azeotropic conditions.

## 922: DIHEXYL KETONE

Tridecanone-7.
Oenanthone. (old, somewhat confusing name).
Di-*n*-hexylketone.

$CH_3—(CH_2)_5—CO—(CH_2)_5—CH_3$

$C_{13}H_{26}O = 198.35$

Leafy crystals or colorless crystalline mass. Sp.Gr. (liquid) 0.82. B.P. 264° C.
M.P. 33° C.

Insoluble in water and Propylene glycol, soluble in alcohol and oils.

Peculiar, warm-herbaceous-floral odor with a woody undertone. The odor has sometimes been compared to that of the "Strawberry-tree" (Mediterranean Arbutus), at other times it seems that the observer has great difficulties in describing the odor in common terms.

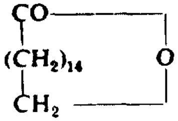
Finds but a little use in perfume compositions. It acts as a fixative – modifier with Coumarin, Benzophenone, Acetanisole etc. in New Mown Hay, Fougère, and other fragrance types.

Prod.: (many methods), e. g.: from Hexyl magnesium chloride and Heptyl nitrile (Hexyl cyanide).

1-173; 26-504; 31-80; 61-67; 66-517; B-I-715;

## 923: DIHYDROAMBRETTOLIDE

Hexadecanolide.
Cyclohexadecanolide.
*16*-Hydroxyhexadecanoic acid, Lactone.
(various isomers are known and have been manufactured).



$C_{16}H_{30}O_2 = 254.42$

Opaque crystalline mass, melting at 36° C. to a viscous or oily colorless liquid.
Sp.Gr. (liquid) 0.94. B.P. 294° C.

Insoluble in water, soluble in alcohol and oils.

Typical musky, sweet odor of great tenacity and fixative power. When compared to Ambrettolide, the DHA is less floral, somewhat weaker and lacks the radiant beauty of the Ambrettolide. The animal notes are slightly more perceptible in the DHA, and it should not be considered as a cheaper replacement for Ambrettolide.

With the appearance of newer macrocyclic musks (such as the Oxahexadecanolides) there is a good possibility that Dihydroambrettolide may be by-passed on the perfumer's shelf. The Oxahexadecanolides are now available at 3 to 10 times lower cost than Dihydroambrettolide.

DHA finds still some application in perfume compositions as a fixative with clean musky, slightly animal and floral undertones, and excellent performance in alcoholic solutions, and on the human skin. It may support delicate floral notes as well as typical Ambre notes or discrete Civet/animal tones, and it blends excellently with the purest Methylionones, Vetiver derivatives and aldehyde blends.

This chemical finds occasional use in flavor compositions, but the author is of the opinion that Ambrettolide and Cyclopentadecanolide are far superior for this purpose (mellowing and "rounding-off").

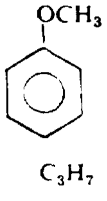
Prod.:

1) from Cyclohexadecanone with "Caro's acid ($H_2SO_5$) followed by hydrogenation.
2) by Cyclization of *omega*-Hexadecanoic acid.

5-204; 86-43; 156-250; 4-60; 86-58; (various patents).

## 924: DIHYDRO ANETHOLE

*para-n*-Propyl anisole.
*para*-Propyl methoxybenzol.
(see also *para*-Cresol propylether).



$C_{10}H_{14}O = 150.22$

Colorless liquid. Sp.Gr. 0.94.
B.P. approximately 225° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-herbaceous, quite powerful odor, less candylike and more dry, almost woody, as compared to Anethole. The overall impression is that of a "clean" odor, not as "round" and "full" as Anethole, yet overall "anisic" of type.

The taste is sweet and typical anisic, yet not as intensely sweet ("candy-sweet") as Anethole, and it lacks the typical Anethole feature of a very wide margin of concentration in application, particularly in flavor compositions. An overdose of Dihydroanethole is usually very perceptible and conspicuously unpleasant.

The material is more stable in soap than Anethole.

It finds some application in perfume compositions, particularly in low-cost masking odors for industrial purposes, detergent perfumes, household fragrances, etc.

It is used in flavor compositions for Licorice, Rootbeer, Birchbeer, Spice blends, Vanilla imitation, Wintergreen, etc.

Concentration in the finished consumer product is normally about 5 to 70 ppm.

G.R.A.S. F.E.M.A. No.2930.

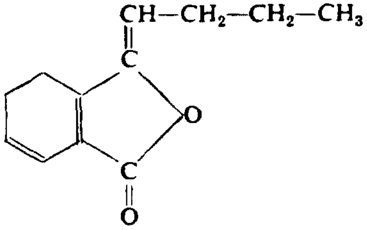
Prod.:

1) by hydrogenation of Anethole.
2) by methylation of *para*-Propyl phenol.

31-147; 90-420; 90-423; 106-132; (Givaudan Corp. info. & data). (U.O.P. Chem. Co. Div. of U.O.P. Inc.).

## 925: DIHYDRO-n-BUTYLIDENE PHTHALIDE

"Ligustilide".
Do not confuse this material with "Ligusticum lactone" (see monograph: *n*-Butylidene phthalide).



$C_{12}H_{14}O_2 = 190.24$

Colorless or very pale yellowish or straw-colored, oily liquid. B.P. 290° C.

Practically insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Very powerful, warm-spicy-herbaceous and sweet odor of excellent tenacity.

In concentrations below 5 ppm the flavor is sweet, warm-spicy, herbaceous, often classified as "soup-like". There is a certain resemblance to some of the characteristic notes of Opopanax.

The title lactone has been suggested for use in flavor compositions, mainly spice- and condiment blends for meat, soups, dressings, sauces, etc. It could also be used in the artificial reconstruction of Celery- and Lovage extracts (oleoresins or oils).

Although the title material and a number of homologues and related chemicals have been identified in natural products, already since long used in food flavoring, the subject material has not been included in the American G.R.A.S. list. It is possible that their chemical relationship to the Coumarins may cause some serious consideration before the authorities will underwrite the safe use of these materials in food flavors. Most conceivably, they will eventually be classified as "safe" when used at concentrations below a certain, specified level.

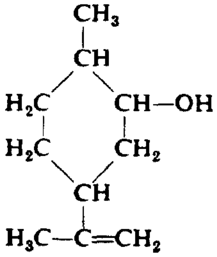
Prod.: from *n*-Valerophenone-*2*-carboxylic acid and Formic acid, followed by controlled hydrogenation of the resulting, unsaturated lactone (Ligusticumlactone).

90-626;

## 926: DIHYDRO CARVEOL

*6*-Methyl-*3*-*iso*-propenyl cyclohexanol.
*para*-Menth-*8*-(*9*)-en-*2*-ol.
Tuberol (Naarden).
Tuberyl alcohol.
•Carhydranol (IFF, Holland).

NOTE: The commercial product is usually a mixture of several stereoisomers. The *dextro*- is the desirable odor type, while the *laevo*- is less so.



$C_{10}H_{18}O = 154.25$

Almost colorless or pale straw-colored liquid, slightly viscous or oily (changes with age). Sp.Gr. 0.93. B.P. 225° C.

The *dextro*-isomer has a woody-floral odor, somewhat sickening-sweet, while the *laevo*-isomer is rather unpleasant, slightly gassy, rather nauseating-animal, resembling the odor of Chenopodium (Wormseed) oil.

Sweet-woody, somewhat spicy, warm taste, in higher concentrations slightly burning, peppery, also with a vague resemblance to Caraway.

Occasionally used in perfume compositions, mainly as a trace ingredient in heavy floral types, Gardenia, Tuberose, and in Geranium bases, woody complexes, etc. It blends well with the Ionones, Sandalwood oil, the "Rose" alcohols, etc.

This alcohol finds more use in flavor compositions, mainly for imitation Pepper, Caraway, Mint (compositions), Spice blends and in various Liqueur flavors.

The concentration in alcoholic beverages may be as high as 500 ppm.

G.R.A.S. F.E.M.A. No.2379.

Prod.: by reduction of Carvone and separation of the isomers.

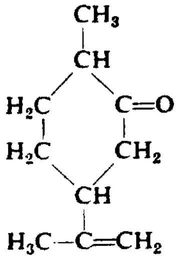
4-43; 26-504; 86-44; 88-97; 158-216;
B-VI-63; 36-366; 31-25;

* This name also used for hydrogenated CARDANOL, obtained from Cashewnut shell oil.

## 927: cis-DIHYDRO CARVONE

*1*-Methyl-*4*-*iso*-propenyl cyclohexanone-*2*.
*cis*-*laevo*-Dihydrocarvone.
*cis*-*para*-Menthen-*8*(*9*)-one(*2*).

(*cis*-):



$C_{10}H_{16}O = 152.24$

Almost colorless or pale straw-colored liquid. Sp.Gr. 0.93. B.P. 222° C.

Insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, powerful and diffusive odor, similar to that of *laevo*-Carvone, but slightly milder, less pungent, sweeter and in dilution less "medicinal".

Its use is mainly in flavor compositions, where it finds a place as a component of artificial Spearmint oil. It has earlier been reported as being a component af natural Spearmint oil.

Prod.:

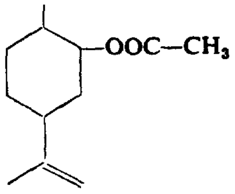
1) by Isomerization of Limonene oxide.
2) from Dihydrocarveol by oxidation – or
3) from Carvone by reduction.

G.R.A.S. (pending, 1967).

4-43; 26-504; 86-44; 89-244; B-VII-83;

## 928: DIHYDRO CARVYLACETATE

*para*-Menth-*8*-(*9*)-en-*2*-yl acetate.
*6*-Methyl-*3*-*iso*-propenyl cyclohexanyl acetate.
Tuberyl acetate (Naarden).
Carhydrine (I.F.F.-Holland).



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.
Sp.Gr. 0.96.

Sweet, slightly minty, floral, rosy odor with a herbal undertone.

Finds a little use in perfume compositions, mainly in sophisticated floral bases.

Used in flavor compositions for imitation Spearmint, for Spice blends, Fruit complexes, Mint compositions, Berry types, etc.

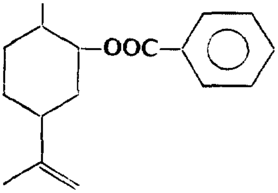
Prod.: by Acetylation of Dihydrocarveol.

G.R.A.S. F.E.M.A. No.2380.

4-43; 90-294;

## 929: DIHYDRO CARVYL BENZOATE

Tuberyl benzoate (Naarden).
NOTE, see below.



$C_{17}H_{23}O_2 = 259.37$

Colorless viscous liquid. B.P. 301° C.
Sp.Gr. 1.03.

Insoluble in water, soluble in alcohol, miscible with oils.

Peculiar dry-musty, almost Ambergris-like odor of excellent tenacity.

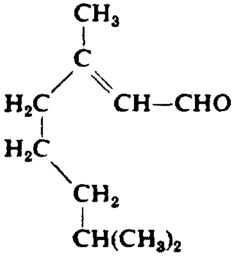
Finds some use in perfume compositions, particularly in Citrus type Colognes as a modifier in the fixative complex, where it blends excellently with Labdanum products, ets.

86-44; 88-99;

NOTE: The name "Cardanyl benzoate" has been given to the benzoate of an alcohol isolated from the Cashew nut shell oil, and it has also been used for the title material, the corresponding alcohol sometimes being called "Carhydranol", the name thus implying a relationship to the hydrogenated alcohol, "Cardanol". The two materials are chemically entirely different.

## 930: DIHYDRO CITRAL

*3,7*-Dimethyl-*2*-octen-*1*-al.



$C_{10}H_{18}O = 154.25$

Almost colorless, mobile liquid.

Rather sharp, minty and "terpeney" odor, not exactly pleasant.

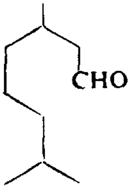
Of very little interest in perfumery.

Not used in flavors.

4-43; 86-44;

## 931: DIHYDRO CITRONELLAL

"Virisal" (Virisacetal – see next).
Citral W. (Hoffmann-laRoche).
*3,7*-Dimethyl octanal.
An aldehyde corresponding to Tetrahydro geraniol.



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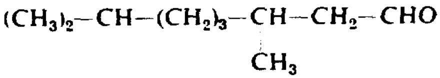


$$(CH_3)_2{-}CH{-}(CH_2)_3{-}\underset{\substack{|\\ CH_3}}{CH}{-}CH_2{-}CHO$$

$C_{10}H_{20}O = 156.27$

Colorless slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, fresh-green lemony-sharp odor with a floral, Lime-like note. Overall bearing some resemblance to the odor of Citral, but lacks the sweetness of that aldehyde. It resembles Gerano-nitrile in odor to a remarkable degree.

Of fairly recent date of development, this aldehyde has already found extensive use not only as a replacement for Citral – in part or in full – but also generally as a fresh-citrusy note of greater stability than Citral.

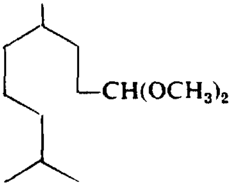
Being a completely saturated aldehyde, it has less tendency to deterioration under alkaline conditions, and will not polymerize.

Not yet specifically listed as G.R.A.S. in the U.S. Federal Register, there should be a good chance that this chemical may be permitted in flavors. Citral is, however, fairly stable in acid media (the predominant condition in Lemon flavors), and produces a more natural Lemon note.

(H.-laRoche data sheet).
4-43; 4-142; 36-368; 86-44; 158-115;

## 932: DIHYDROCITRONELLAL DIMETHYLACETAL

*3,7*-Dimethyloctanal-dimethylacetal.
"Virisacetal".



$C_{12}H_{26}O_2 = 202.34$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 243° C.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, rosy-green, foliage-type, slightly floral odor with ethereal notes.

Overall not very powerful.

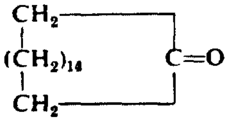
Has been suggested for use in perfume compositions, but does not seem to have gained much interest among the creative perfumers.

Prod.: from Dihydrocitronellal and Methanol.

4-43; 36-368;

## 933: DIHYDROCIVETTONE

Cycloheptadecanone.



$$\begin{array}{ll} CH_2 & \\ | & \\ (CH_2)_{14} & C{=}O \\ | & \\ CH_2 & \end{array}$$

$C_{17}H_{32}O = 252.44$

Colorless viscous oil. Insoluble in water, soluble in alcohol and oils.

Faint, animal-musky odor, sweet, and slightly woody with good tenacity. Compared to Civettone, the DHC is considerably weaker and less characteristic "clean-animal-musky" in its overall performance.

The effect in alcoholic solution on human skin is also poorer than in the case of Civettone.

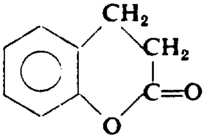
This macrocyclic ketone is of little more than academic interest.

Prod. by catalytic reduction of Civettone.

86-46; 156-250;

## 934: DIHYDROCOUMARIN

*3,4*-Dihydrocoumarin.
Hydrocoumarin.
*1,2*-Benzodihydropyrone.
Tonka-mel (Norda).
Toncainol (Lautier Fils).
Melilotine (Greeff).
*ortho*-Hydroxydihydrocinnamic acid, Lactone.
Melilotic acid, Lactone.



$C_9H_8O_2 = 148.16$

Viscous, almost colorless liquid, solidifying in the cold, melting at 23° C. Sp.Gr. 1.19. B.P. 272° C.

Slightly soluble in water, soluble in alcohol, miscible with oils.

Sweet-herbaceous, nutlike, haylike odor, usually described as "coumarinic" or "tobacco-like".

When this material is compared to Coumarin, it appears that Coumarin is actually stronger in practical use (soap, etc.) and outperforms the DHC on tenacity. Yet, the Dihydrocoumarin has been advertised as being two to three times stronger than Coumarin. The author has seen no practical proof of this statement.

The taste is sweet, caramellic-nutlike, herbaceous. It is very close to Coumarin as far as type is concerned. The Dihydrocoumarin was recommended as a "Coumarin substitute" in the first few years after the ban on Coumarin as a food flavor chemical in the U.S.A. It has a little of Coumarin's ability to fortify the flavor of Vanilla, and is often used for that purpose. It supplies a rich "body" or undertone in a flavor and blends well with most Spices, Nut-flavor chemicals, etc.

Its use in perfumery has remained very limited, since it did not offer any superior effects as compared to Coumarin.

Used in imitation Butter, Caramel, Coconut, Cherry, Cinnamon, Cream-Soda, Floral, Fruit, Nut, Rum, Tonka, Vanilla, etc. and in Spice blends, Rootbeer formulations, Liqueur bases, etc. Concentration is about 50 ppm in finished candy, and as high as 75 to 80 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2381.

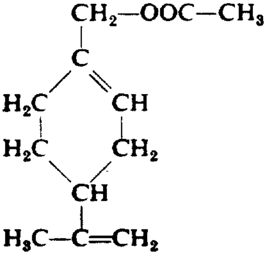
Prod.:

1) by reduction of Coumarin with a Nickel catalyst.
2) by Lactonization of *ortho*-Chlorohydrocinnamic acid.

4-43; 7-211; 30-256; 31-166; 86-44; 90-959; 95-194; 96-180; 106-66; 156-131; 140-155;

## 935: DIHYDROCUMINYL ACETATE

Perillyl acetate.
*1,8-para*-Menthadien-7-yl acetate.
*4-iso*-Propenyl-*1*-cyclohexenyl acetate.
Menthadiene-7-carbinyl acetate.



$C_{12}H_{18}O_2 = 194.28$

Almost colorless or pale yellowish oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, spicy odor, suggestive of Dill and Spearmint, but with a very diffusive and refreshing, almost fruity note (in proper dilution).

Has been suggested for use in perfumery, e. g. in the reconstruction of certain essential oils (Bergamot, etc.).

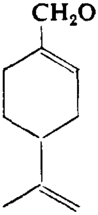
Finds some use in flavor compositions, mainly as a component of artificial Spearmint, and in Spice and condiment flavor blends.

Prod.: by direct esterification of Dihydrocuminyl alcohol (see next).

90-295;

## 936: DIHYDROCUMINYL ALCOHOL

*1,8-para*-Menthadien-7-ol.
*4-iso*-Propenyl-*1*-cyclohexene carbinol.
*1*-Hydroxymethyl-*4-iso*-propenyl-*1*-cyclohexene.
Hydrocumin alcohol.
Perillyl alcohol.
Perilla alcohol.
"*iso*-Carveol".
Menthadiene-7-carbinol.



$C_{10}H_{16}O = 152.24$

Colorless or pale yellowish, oily liquid.
B.P. 228° C. Sp.Gr. 0.95.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-herbaceous, slightly woody-oily, floral (petal-like) odor.

Woody-minty, slightly oily, but not very sweet taste. Very powerful.

Occasionally used in perfume compositions, mainly as a trace ingredient in artificial flower absolutes or essential oils. It imparts pleasant and natural Lily-like notes in conjunction with Hydroxycitronellal or Bucinal, lends green-floral notes to Muguet or Narcissus, and petal-like effect in Rose, etc.

Used in flavor compositions for imitation Citrus, Vanilla, Mint (mainly Spearmint) and in Fruit compositions.

The concentration in the finished consumer product may vary from 0.5 to 50 ppm.

G.R.A.S. F.E.M.A. No.2664.

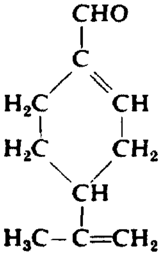
Prod.:

1) by catalytic reduction of Dihydrocuminyl aldehyde (see next).
2) by oxidation of *beta*-Phellandrene, followed by reaction of the Glycol with diluted sulfuric acid to yield Dihydrocuminyl alcohol and Tetrahydro cuminyl alcohol.

7-194; 7-229; 65-47; 88-111;

## 937: DIHYDROCUMINYL ALDEHYDE

Perilla aldehyde.
*para*-Menthadien-*1,8(9)*-al-*7*.
*4-iso*-Propenyl cyclohexen-*1*-aldehyde.
Dihydro cuminic aldehyde.



$C_{10}H_{14}O = 150.22$

Pale yellowish oily liquid. B.P. 237° C. Sp.Gr. 0.96.

Almost insoluble in water, soluble in alcohol and oils.

Powerful fatty-spicy, oily-herbaceous odor, reminiscent of Dill, Cumin and Gingergrass (green-oily, weedy notes).

Sweet-herbaceous, slightly spicy taste in extreme dilution.

Occasionally used in perfume compositions and in artificial essential oils, such as Bergamot, Caraway, Spearmint, etc.

Introduces fresh-floral-green notes in Jasmin, Tuberose, Narcissus, etc.

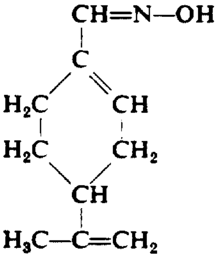
Finds a little use in flavor composition as a fortifier and modifier in Spice blends, Dill flavorings, etc.

Prod. by isolation from Japanese Perilla leaf oil.

31-41; 31-61; 65-342; 77-205; 89-115;
see also 104-520;

## 938: DIHYDROCUMINYL ALDEHYDE-anti-ALDOXIM

"Perillartine" ("Peryllartine").
*laevo*-Perilla aldehyde-*alpha-anti*-aldoxim.



$C_{10}H_{15}NO = 165.24$

White powder. Slightly soluble in water, soluble in alcohol.

Practically odorless.

Intensely sweet taste. Estimated sweetening strength is about 2000 times that of cane sugar, compared in 5% aqueous solution of the cane sugar (against 25 ppm Peryllartine in water).

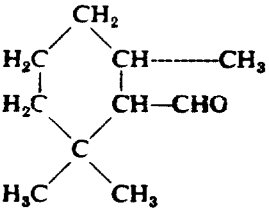
Developed in the early 1920's, this chemical has been in use in Japan almost ever since, but has never achieved much popularity outside of that country.

Prod.: from Dihydrocuminyl aldehyde and Hydroxylamine.

1-924; 100-786;
see also: C. F. Walton: Internat. Critic. Tables, Vol. 1, 1926 (New York).

## 939: DIHYDRO CYCLOCITRAL

Exists in *cis*- and *trans*-isomer.
Commercial grade is mainly *trans*-.
The corresponding alcohol is: Dihydrocyclogeraniol (see next).



$C_{10}H_{18}O = 154.25$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.
Sp.Gr. 0.91. B.P. 188° C.

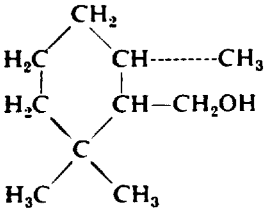
Camphor-like, cool-herbaceous odor.

Of very little interest to perfumers.

86-44;

## 940: DIHYDRO CYCLOGERANIOL

Exists in *cis*- and *trans*-isomer.



$C_{10}H_{20}O = 156.27$

Colorless, slightly oily liquid. Sp.Gr. 0.92.

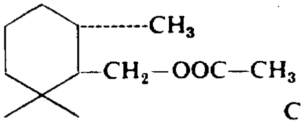
Very slightly soluble in water, soluble in alcohol and oils.

Weak, woody-floral odor with camphoraceous undertone.

Of very little interest to the perfume industry.

86-44;

## 941: DIHYDRO CYCLOGERANYL ACETATE



$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

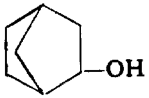
Mild, oily-rosy, fruity and somewhat green odor. Much weaker than Geranyl acetate, and not as Apple-like.

Sweet, rosy-fruity taste with a slightly bitter undertone (unless very highly diluted).

Has been suggested for use in perfume compositions as a modifier for Geraniol-Geranylacetate, but its lack of power makes it rather undesirable or uninteresting.

## 942: DIHYDRO CYCLOL

Diheptol.
Bicyclo (*2:2:1*) heptanol.
Norborneol.



$C_7H_{12}O = 112.17$

Colorless or white crystals. M.P. 150° C. B.P. 214° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild and relatively sweet woody-piney odor of moderate tenacity.

This alcohol, which is commercially available as a result of the increasingly popular Diels-Alder adduct-synthesis, has found extensive use in perfumery as a major ingredient in low-cost fragrances for household products, detergents, etc.

Partly as a companion to *iso*-Bornylacetate, partly as a background for Lavandin-type fragrances, it enhances these odors and gives the desirable "lift" in fragrances where tenacity is often unwanted, and where immediate freshness, radiation, diffusive power are the prerequisites.

RELATED PRODUCTS:

(Homo-): The next higher homologue, *2*-Hydroxymethylbicyclo (*2:2:1*) heptane, is also known. It is prepared from the Acrolein-Cyclopentadiene adduct by reduction.

(Aldehyde): The aldehyde (adduct) itself, Bicyclo (*2:2:1*) hept-*5*-ene-*2*-aldehyde is also known as a perfume chemical, and its acetal is used under a trade name.

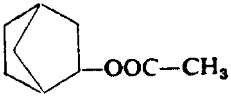
(Acetal): This acetal has an enormously diffusive effect and finds limited use in Pine needle fragrances where its sweet-green odor at very low concentrations (often less than 0.2% in the perfume oil) appears to be interesting not only from an economical point of view.

(Ester): The title material is prepared from Cyclopentadiene plus Vinylacetate, followed by reduction, which yields the Acetate of the subject material (Acetate – see next). Hydrolysis of the acetate yields the alcohol Norborneol.

67-340;

## 943: DIHYDRO CYCLYLACETATE

Diheptyl acetate.
Norbornyl acetate.
Bicyclo (*2:2:1*) heptanyl acetate.



$C_9H_{14}O_2 = 154.21$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Refreshing light, woody-piney odor with mildly herbaceous-fruity undertones.

This ester has found considerable use in perfume compositions, particularly in the low-cost, large-volume fragrances for household products, detergent perfumes, room sprays, insecticide masking odors, etc.

It is commercially available and it is prepared from very inexpensive readily available industrial chemicals.

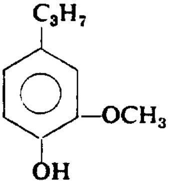
Related materials are briefly mentioned in the previous monograph under the head name: Dihydro cyclol.

Prod.: By Diels-Alder adduct reaction from Cyclopentadiene and Vinylacetate followed by reduction of the unsaturated alcohol ("Cyclol").

67-340;

## 944: DIHYDROEUGENOL

*n*-Propyl guaiacol.
Eugenol M.
*1*-Propyl-*3*-methoxy-*4*-hydroxybenzene.
*2*-Methoxy-*4*-propylphenol. (sometimes called).



$C_{10}H_{14}O_2 = 166.22$

Almost colorless oily liquid. Sp.Gr. 1.04. B.P. 250° C.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-spicy, sweet and slightly floral-balsamic odor, reminiscent of Eugenol, but milder and sweeter than this.

Discolors less in soap than Eugenol, but only when measured weight/weight – not considering equal odor strength (it takes more DHE than Eugenol to produce a certain amount of spicy odor).

Occasionally used in perfumery as a substitute for Eugenol when Eugenol seems to produce a problem with possible discoloration.

However, since DHE is manufactured from Eugenol and weaker than Eugenol, it is not very economical in use.

Prod.: by catalytic reduction of Eugenol with Palladium or Platinum black catalyst.

4-44; 68-973; 158-164; 90-415;

## 945: DIHYDROFARNESOL

Although the title material theoretically exists, the author is inclined to believe that confusion with Dihydrofarnesene, or Hexahydrofarnesol could have caused mention of or interest in the title material.

$C_{15}H_{28}O = 224.39$

Almost colorless, slightly oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet and mildly floral odor with a soft, woody undertone and good tenacity. The odor is even milder than that of Farnesol, and the tenacity is poorer. The title material does not seem to show the same tendency of "growing" in odor power in a composition, such as can be observed with Farnesol, etc.

The alcohol has been suggested for use in Lilac, Honeysuckle and other floral perfume compositions.

Prod. from Farnesol. (Presumably absolete).

4-44; 88-238;

## 946: DIHYDRO GERANIOL

*d,l*-Citronellol.
Citronellol (racemic).

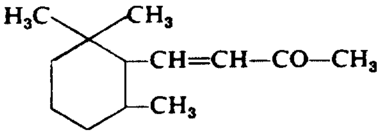
This material represents a no longer demanded type of Citronellol, made by reduction of Geraniol.

The commercial product contained significant amounts of Dimethyl octanol and was not a well-defined perfume chemical.

See monograph: CITRONELLOL.

## 947: cis-DIHYDRO IONONE

*2,6,6*-Trimethyl cyclohexyl-*1*-butenone-*3*.
(Commercial product is not pure).



$C_{13}H_{22}O = 194.32$

Colorless to pale yellowish oily liquid.
B.P. 240° C. Sp.Gr. 0.92.

Almost insoluble in water, soluble in alcohol and oils.

Woody and slightly floral odor, considerably weaker than the odor of *alpha-* and *beta-*Ionones.

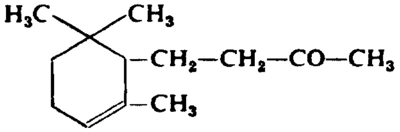
Has been suggested for use in perfume compositions as a modifier for the regular Ionones, and as a new variety of the floral Ionone type.

It has never become a very common or freely available chemical and does not seem to be much in demand.

Prod.:
1) from Dihydrocyclocitral and Acetone by condensation.
2) by condensation of Citronellal and Acetone, followed by cyclization.

86-45; 96-168;

## 948: DIHYDRO-alpha-IONONE



$C_{13}H_{22}O = 194.32$

Colorless to pale yellowish oily liquid. Almost insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.92. B.P. 234° C.

Rather "thin" oily-woody odor, somewhat "gassy" and weaker than *alpha*-Ionone with respect to Violet-note.

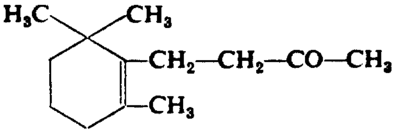
Of very little interest to the perfumer.

Prod.: by partial hydrogenation of *alpha*-Ionone.

4-44; 31-94; 86-45; 96-168;

## 949: **DIHYDRO**-beta-**IONONE**

*4*-(*2*,*6*,*6*-Trimethylcyclohexen-*1*-yl)-butan-*2*-one.



$C_{13}H_{22}O = 194.32$

Colorless to pale yellowish oily liquid. Practically insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.93. B.P. 236° C.

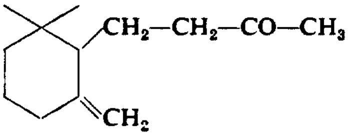
Of little or no interest to the perfumer.

This material is generally described as inferior to *beta*-Ionone with respect to power and odor beauty.

4-44; 86-45;

## 950: **DIHYDRO**-gamma-**IONONE**

*4*-(*2*-Methylene-*6*,*6*-dimethylcyclohexyl)-butan-*2*-one.
(This monograph describes the commercial mixture of isomers).



$C_{13}H_{22}O = 194.32$

Almost colorless or very pale straw-colored oily liquid. Sp.Gr. 0.91. B.P. 241° C.

Insoluble in water, soluble in alcohol and oils.

This material, when marketed commercially, will usually consist of a mixture of several isomers. It has been claimed that not all of them are of interesting odor.

The most appreciated odor type is that of Ambregris, and the title material is normally described as having such odor type. A general odor description of Dihydro-*gamma*-ionone is therefore of little value.

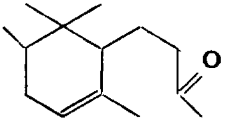
This ketone is occasionally used in compositions aiming at the complex odor of Ambregris. It is said to be a major component of one or more well-known Ambregris specialties, but the secret of its odor lies still in the proper isomer-ratio, just as it often does for the Methylionones and Ionones.

Prod.: by controlled hydrogenation of *gamma*-Ionone, normally with a platinum catalyst, or a Raney-nickel catalyst.

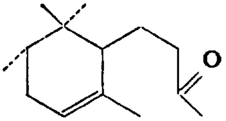
4-44; 86-45; 156-211;

## 951: **DIHYDRO**-alpha-**IRONE**

This monograph includes one isomer:
DIHYDRO-*iso*-*alpha*-IRONE.
*1*-(*2*,*5*,*6*,*6*-Tetramethyl-*2*-cyclohexenyl)-butan-*3*-one.



Dihydro-*alpha*-irone
(*cis*-isomer)



Dihydro-*iso*-*alpha*-irone
(*trans*-isomer)

$C_{14}H_{24}O = 208.35$

Almost colorless oily liquid. B.P. 244° C.
Sp.Gr. 0.93.

Practically insoluble in water, soluble in alcohol and oils.

These ketones, rarely offered individually in a pure state, have been manufactured on a limited scale but are not commonly available. They were developed in an attempt to find more stable versions of the Irone theme, but they do not seem to distinguish themselves with greater stability.

From an odor point of view, they are rather disappointing, being weaker or milder than *alpha*-Ionone and resembling that ketone in character.

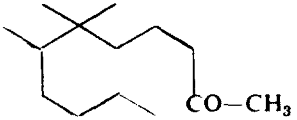
They are mentioned in this book mainly to supply example of some of the numerous possible isomers of Dihydro irone and other relatives of Irone, very few of which have ever achieved popularity or use in creative perfumery.

Prod.: *from alpha*-Irone by hydrogenation in presence of Raney-nickel catalyst. The two subject isomers are both present in the reaction mixture.

12-47; 86-66; 86-68; 89-406;
See also: *alpha*-Irone.

## 952: **DIHYDRO**-beta-**IRONE**

A mixture of up to 13 isomers and homologues:



$C_{14}H_{24}O = 208.35$

Almost colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Dry and rather hard odor, generally considered undesirable, yet reminiscent of *beta*-Ionone in overall type.

This ketone has been manufactured on a very limited scale, but has, to the author's knowledge, not found any significant application in perfumery.

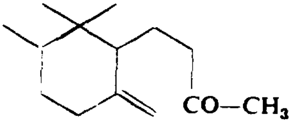
See also comments under Dihydro-*alpha*-irone.

Prod.: by hydrogenation of *beta*-Irone. The reaction mixture contains not only the title material, but also Tetrahydro irones and related materials.

12-47; 86-68; 89-406;

## 953: **DIHYDRO**-gamma-**IRONE**

A mixture of at least two isomers, including Dihydro-*iso-gamma*-irone.



$C_{14}H_{24}O = 208.35$

Almost colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

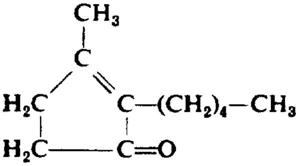
Although this ketone resembles *alpha*-Irone from an olfactory point of view, it has failed to interest the perfumers, partly because it is very unstable, partly because it seems to be difficult to produce in a pure state and consistent quality.

It is produced by hydrogenation of *gamma*-Irone.

12-47; 86-66; 86-68; 89-406;

## 954: DIHYDRO JASMONE

*2*-Pentyl-*3*-methyl-*2*-cyclopenten-*1*-one.
*3*-Methyl-*2*-(*n*-pentanyl)-cyclopenten-*2*-one-*1*.
Methyl-*3*-pentyl-*2*-cyclopenten-*2*-one-*1*.
Tetrahydro pyrethrone.
"*iso*-Jasmone" (sometimes called).



$C_{11}H_{18}O$ = 166.27

Almost colorless, slightly oily liquid.

Very slightly soluble in water, soluble in alcohol and oils. Moderately soluble in Propylene glycol.

Sp.Gr. 0.92. B.P. 230° C.

Intensely floral and fresh odor with fruity and somewhat Myrrh-like undertone. There is considerable difference in odor between products from different manufacturers. The name Dihydro jasmone is also applied to chemicals which should truly be called Dihydro-*iso*-jasmone. Dihydro jasmone is often described as the "closest to *cis*-Jasmone in odor". In proper dilution it has a pleasant, sweet, herbaceous-floral taste which is easily twisted towards a fruity note in presence of traces of fruity chemicals. It has an excellent softening effect upon the overly "chemical" fruit materials.

Widely used in perfume compositions, not only for artificial Jasmin and Bergamot, but in general as a floralizer in the more fruity-floral fragrance types: Ylang, Lily, Tuberose, Magnolia, etc. and it introduces a pleasant undertone in Citrus type fragrances.

Finds some use in flavor compositions, often as a "mellowing" agent in very "artificial" or "chemical" flavor compositions. The fruity note blends well into Banana, Peach, Apricot, Pear, etc.

Prod.:

1) Hexylbromide + Levulinic ester to yield a Lactone, which is reacted with Polyphosphoric acid or Phosphorpentoxide to produce Dihydrojasmone.
2) From Methyl cyclopentenolone (an isomer of Cyclotene).
3) by hydrogenation of *trans*-Jasmone (by-product from *cis*-Jasmone synthesis) and by many other methods.

4-44; 5-156; 30-420; 67-101; 89-365; 89-366; 86-45; 158-220; Naarden's data sheet: one of "Naarden's Seven" (1966); 156-224;

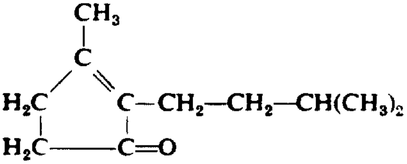
## 955: DIHYDRO-iso-JASMONE

The commercial products under this name are usually mixtures of several components, mainly:

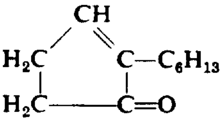
1) Methyl-*3*-*iso*-amyl-*2*-cyclopenten-*2*-one-*1*, and:
2) *n*-Hexyl cyclopentenone.

The former represents the preferred odor type.

(1)



(2)



$C_{11}H_{18}O$ = 166.27

Pale straw-colored liquid. Boiling range 219 to 238° C. Sp.Gr. 0.91.

The odor is more fruity, less floral than that of Dihydro jasmone (see previous monograph).

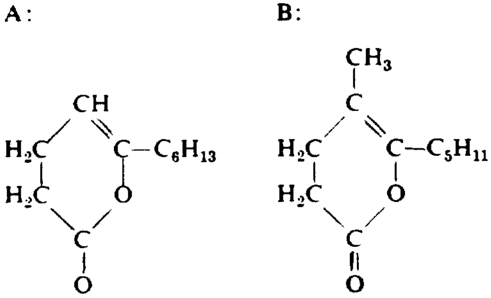
This material is used in perfume compositions for its floral effect mainly in such florals where a distinctly fruity note is acceptable or even desirable ("White Shoulders" - type of fragrance). It blends well with the heavy fruity notes from Undecanolide and the musky notes from Ethylene brassylate or newer synthetic musks. Ionones and particularly Methylionones supply very good background for this Jasmone-derivative.

The use in flavors is very small, since the taste of this mixture is inferior to that of Dihydro jasmone and other single chemicals.

Prod.: from *iso*-Jasmone by hydrogenation (*iso*-Jasmone contains several isomers).

156-223;
See also "Naarden News", Vol. 17, No. 175, October 1966 (U.S. edition).

## 956: DIHYDRO JASMONE LACTONE



$C_{11}H_{18}O_2 = 182.27$

Faintly straw-colored or almost colorless oily liquid.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Heavy floral, but also fatty (Coconut-fatty) and waxy odor. The floral notes resemble those of Gardenia (undertones) and Tuberose, but the beauty of these notes is somewhat marred by the interference of fatty notes.

Powerful, fatty, Peach-like taste in extreme dilution.

Overall not a very interesting perfume material.

It represents an intermediate in the manufacture of Dihydrojasmone.

Prod.:
A) from Hexylbromide and Levulinic ester (Ethyl levulinate).
B) from Methylamylcyclopentanone by oxidation and Hydrolysis followed by Lactonization of the hydroxyacid.

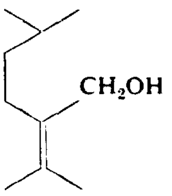
31-174; 156-224;

## 957: iso-DIHYDRO LAVANDULOL

A: *2,6*-Dimethyl-*3*-Hydroxymethyl-*2*-heptene.
*5*-Methyl-*2*-*iso*-propylidene-*1*-hexanol.
B: *iso*-Dihydrolavandulyl alcohol.
*2,7*-Dimethyl-*6*-hydroxy-*4*-octene.
*2*-Methyl-*6*-*iso*-propyl-*4*-hexenol.

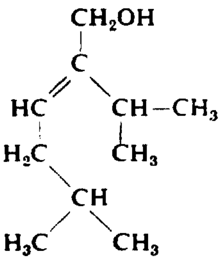
Structures for commercially available materials have been given with considerable variations:

A:



This structure corresponds to above synonyms A.

B:



Structure sometimes given

$C_{10}H_{20}O = 156.27$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils. Somewhat soluble in Propylene glycol. B.P. 201° C.

Refreshing herbaceous-minty, also Pulegol-like, Lavender type odor of moderate tenacity.

Herbaceous, minty-Lavender-like taste, but rather bitter at concentrations higher than 20 ppm.

This material, developed at the time when Lavandulol was still relatively expensive, offers quite refreshing notes at low cost, but it does not substitute for Lavandulol in artificial Lavender or Lavandin oils. The title alcohol finds use in soap and detergent perfumes, room spray fragrances, etc. There is considerable difference in odor between the materials from different suppliers.

Prod.: (several methods) e.g. from 5-Methyl-*2*-*iso*-Propyl hexene-*2*.

(Samples: Fritzsche Bros. Inc., and Takasago Perf. Co. Ltd.).

163-349; "Recherches", 14, 1964, page 47.

## 958: iso-DIHYDRO LAVANDULYL ACETATE

Structure and synonyms:
See previous monograph: *iso*-Dihydrolavandulol.

$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils. Somewhat soluble in Propylene glycol. B.P. 211° C.

Pleasant and refreshing, Lavender-Lavandin-type note. Not as sweet as Linalylacetate. More woody and mildly camphoraceous. Richer and more tenacious than Linalyl acetate.

Herbaceous-fruity taste with bitter undertone.

This ester has been suggested for use in perfume compositions and as a component in artificial Lavandin or Lavender oils. It can be manufactured at a cost well below that of Lavandulyl acetate, which is a preferred item for artificial Lavender oil. However, it does not substitute for the Lavandulylacetate in these artificial oils, unless one is willing to compromise with a situation of scarcity or extreme emergency.

It serves the title ester better that we consider it as a new perfume chemical with its own place and purpose in perfumes. Its low cost permits use in fragrances for household products, etc. including soap perfumes and low-cost cosmetic fragrances.

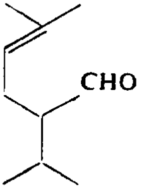
Prod.: by acetylation of *iso*-Dihydrolavandulol (see previous monograph).

(Samples: Fritzsche Bros. Inc. and Takasago Perfumery Co. Ltd.).

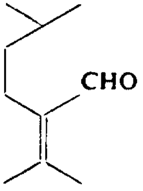
163-349;

## 959: iso-DIHYDRO LAVANDULYL ALDEHYDE

Several structures are given:



or:



$C_{10}H_{18}O = 154.25$

(See also notes under *iso*-Dihydrolavandulyl alcohol).

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful, herbaceous-resinous, slightly minty odor with woody-Lavender-like undertone and moderate to poor tenacity. It is quite possible that the "varnishy" or "resinous" notes derive from Myrcene-derivatives as trace components from the process.

This aldehyde, only a few years on the market, has found some use in fragrances for household products and as a fortifier in Lavender soap perfumes or room spray fragrances, etc. It gives quite refreshing and green effects, and these are very much in demand these years.

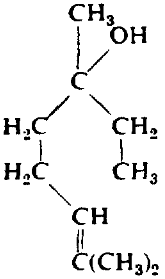
However, its field of application is rather limited, and it does not contribute very unusual notes or effects to a fragrance. Its low cost is among its best assets.

Sample: Fritzsche Bros. Inc.

"Recherches", 1964, vol. 14, page 47.

## 960: DIHYDRO LINALOOL

3,7-Dimethyl-6-octen-3-ol.



$C_{10}H_{20}O = 156.27$

Colorless oily liquid. Sp.Gr. 0.86. B.P. 201° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Comparatively powerful, fresh-floral, citrusy (with emphasis on Lime) and diffusive odor. Less woody than Linalool, more powerful and more Lime-like than Tetrahydro linalool.

An excellent perfume material for fresh-floral fragrance types, as a modifier in Lime and Lime-floral complexes, as a blender in modern soap perfume compositions. More versatile than Linalool and Tetrahydrolinalool, but not quite as discrete as the latter.

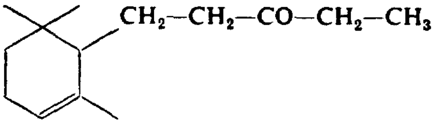
Prod.: by catalytic, partial hydrogenation of Linalool.

4-44; 4-63; 156-238;

## 961: DIHYDRO-alpha-METHYL IONONE

5-(2,6,6-Trimethyl-2-cyclohexenyl)- pentan-3-one.

The commercial product is not a pure, single chemical, but consists mainly of the title material.



$C_{14}H_{24}O = 208.35$

Almost colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild, oily-woody odor of *alpha*-Methyl ionone type, but much weaker.

This ionone has found a little use in perfumery for its pleasant Ionone-effect and greater stability than Methyl ionone.

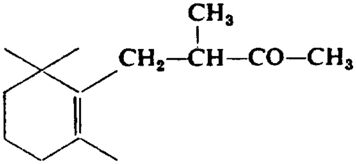
One common disadvantage of the Ionones and Methylionones is their strong tendency to attract Oxygen which in turn may affect the easily oxidizable components in a fragrance composition. The affinity for Oxygen is so pronounced that one can observe a "vacuum" effect in a bottle with Ionone after a short time of storage (unless the bottle was filled with practically no air over the liquid, or if a Nitrogen blanket was provided for protection of the Ionone.

It is only welcome to have materials of Ionone odor effect and without this undesirable side effect. But unfortunately, the title material does not have nearly the power of the conventional Methylionones, and it is therefore not very commonly used.

Prod.: by controlled catalytic hydrogenation of *alpha*-Methyl ionone.

## 962: DIHYDRO-delta-METHYLIONONE

Dihydro-*iso*-methyl-*beta*-ionone.
*delta*-Hydromethylionone.



$C_{14}H_{24}O = 208.35$

Almost colorless or very pale yellowish or straw-colored, viscous liquid. Practically insoluble in water, soluble in alcohol and oils.

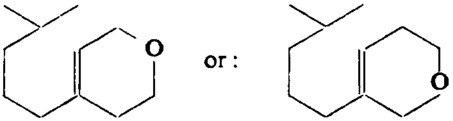
Warm, but rather dry Ambre-gris type odor of good tenacity. The woody and delicately dry notes of *delta*-Methylionone are further refined, but appear less woody, more Ambregris-like.

This Ionone has been suggested for use in perfume compositions where large amounts of dry-sweet Ambregris-notes are called for, as in many modern aldehydic or non-floral types, or in the types developed since "Je reviens", etc. This Ionone performs very well with Ambregris tincture and with Clary Sage absolute, refined Labdanum products or Oakmoss products, Galbanum, terpeneless Juniperberry, etc.

It is rarely offered commercially under its proper chemical name, but it is used by a number of perfume houses with facilities for manufacturing such Ionones themselves.

Prod.: by selective hydrogenation of *iso*-Methyl-*beta*-ionone (so-called *delta*-Methylionone).

## 963: DIHYDRO-4-(or -3)-(4-METHYL-3) (or -2)-PENTEN-1-YL-$\Delta^3$-PYRAN



$C_{11}H_{18}O = 166.27$

Colorless or very light yellowish or straw-colored liquid. Practically insoluble in water, soluble in alcohol and oils.

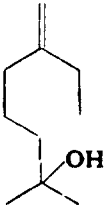
Refreshing and powerful, green-leafy, rosy and sweet odor with a sweet-caramellic, in high concentrations almost "burnt" note, but in dilution pleasantly sweet, slightly fruity. Moderate tenacity.

This material, remotely related to Rose oxide and having one more Carbon atom in its structure, was developed in search of more powerful key chemicals in the rose picture. It is not believed to be a natural component of Rose, but it served a good purpose in the years prior to the commercial production and common appearance of Rose oxides on the perfumery raw material market.

It is not very stable towards exposure to air, seems to resinify and turn darker in color, less pungent in odor. It is most conceivable that the material will become obsolete within a decade or so, mainly in competition with more natural, stable and versatile materials.

## 964: DIHYDRO MYRCENOL

3-Methylene-7-methyloctanol-7.



$C_{10}H_{20}O = 156.27$

Colorless, somewhat viscous oil. Practically insoluble in water, soluble in alcohol and oils.

Powerful, fresh Lime-like, overall citrusy-floral and sweet odor with little or no terpenic undertones.

The material shows some tendency to polymerization, whereby it loses odor and increases in viscosity. With proper inhibitor added, it is fairly stable against such deterioration.

Useful in soap perfumes and as a powerful supporting note under Lime oils in Citrus and Lime-type fragrances. It belongs to a very small group of chemicals that have typical Lime notes without being a hydrocarbon.

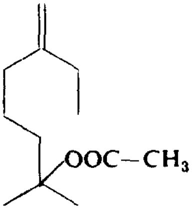
It introduces fresh and powerful, diffusive notes to floral bases, Muguet, Lily, Lilac, Hyacinth, etc., and produces interesting blends with Rose chemicals.

Prod.: by controlled, partial hydrogenation of Myrcenol, see *3*-Methylene-7-methyl-*1*-octen-7-ol.

156-374;
I.F.F. sample.

## 965: DIHYDRO MYRCENYL ACETATE

*3*-Methylene-7-methyloctan-7-yl acetate.



$C_{12}H_{22}O_2 = 198.31$

Colorless mobile liquid. Almost insoluble in water, soluble in alcohol and oils.

Sweet, spicy-herbaceous, fresh and somewhat fruity odor with Bergamot-Lime character. Moderate to poor tenacity.

This ester is more stable than Myrcenyl acetate which tends to polymerize upon standing. It is not quite as powerful and does not give the same effect in a soap (perfume). But it has a different odor character, more citrusy-fresh, more interesting for modern versions of the "Continental" style Citrus-cologne. It will also support the Lime notes in Lime or Lime-Lemon fragrances, a very modern and much demanded type in recent years (1967-68). Novel effects in Jasmin bases are also achieved with this ester.

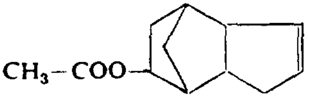
Prod.: by controlled hydrogenation of Myrcenyl acetate, or by Acetylation of Dihydromyrcenol.

See also monograph: *3*-Methylene-7-methyl-*1*-octen-7-ol (Myrcenol).

156-374;
I.F.F. sample.

## 966: DIHYDRO-NOR-DICYCLOPENTADIENYL ACETATE

"Verdyl acetate" (Givaudan Corp.).



$C_{12}H_{14}O_2 = 190.24$

Colorless or almost colorless, viscous liquid. Sp.Gr. 1.08.

Practically insoluble in water, soluble in alcohol and oils.

Powerful herbaceous-green and fresh-woody odor of considerable tenacity.

The virtues of diffusion and tenacity are not often found at the same time in one perfume chemical, and this alone brings the subject ester into limelight of interest. Its stability and low cost contribute to the greater expansion of its field of application including soap and detergent perfumes, air (space) fresheners, etc.

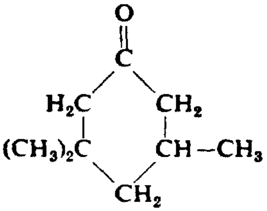
This ester offers excellent opportunities for the creative perfumer who seeks novel notes or more than a "twist" to the conventional notes in modern perfumery. In Chypre, Fougère, Lavender and aldehydic-woody or green-fruity compositions, the subject ester can find use and it can offer quite unique effects.

The trend in modern perfumery (1967-68) seems to be toward an emphasis on green notes, however, a more natural type of greenness, and not always accompanied by Oakmoss and fruity notes.

(Sample and data sheet: Givaudan Corp.).

## 967: DIHYDRO-iso-PHORONE

Sometimes called: *iso*-Phorol (see monograph).
*3,5,5*-Trimethyl cyclohexanone.



$C_9H_{16}O = 140.23$

Colorless oily liquid. B.P. 167° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet, honey-tobacco-like odor with warm-herbaceous undertones. Overall milder, sweeter and less harsh than *iso*-Phorone.

This ketone, rarely offered commercially, is occasionally used in perfume compositions for its Honey-Labdanum effect. It blends excellently with the Phenylacetates, Ionones, Anisylesters, etc. and will, in spite of its comparatively low boiling point, appear mild and sweet, rounding off the more chemical notes of the simple Phenylacetates or the camphoraceous notes in certain types of Labdanum product.

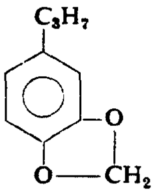
Although the parent, unsaturated ketone (see *iso*-Phorone) is available as a low-cost industrial chemical, there seems to be little interest in the subject material. Yet, interesting effects can be achieved with it in the relatively rare cases where novel tobacco-effects are desired, or variations in Labdanum or "miel" bases are wanted.

Prod.: by catalytic hydrogenation of *iso*-Phorone.

67-193; see also: 67-208; 3-301;

## 968: DIHYDRO SAFROLE

*3,4*-Methylenedioxy propylbenzene.



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils. Very poorly soluble in Propylene glycol. Sp.Gr. 1.07.

Sweet, root-like, floral-anisic odor, warm and somewhat spicy. Weaker than Safrole, often described as "less sassafrassy".

Finds some use in perfumery, partly as a component of artificial Nutmeg, Sassafras and other oils, partly as a sweetener in various fresh or citrusy fragrance types. It blends well with Bergamot, Coumarin, Amylsalicylate, Labdanum, Tolubalsam, etc.

Was suggested as a substitute for Safrole in flavors, but the Dihydro safrole was never approved in the U.S.A. as a food flavor ingredient. Since it is a derivative of Safrole, it does not even have the advantage of a lower price than Safrole.

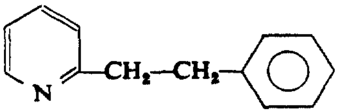
Prod.:

1) by reduction of Safrole with Sodium alcoholate.
2) by catalytic hydrogenation of Safrole.

68-974; 68-977; 72-88; 90-453; 106-133; 140-171;

## 969: DIHYDRO-alpha-STILBAZOLE

Dihydro-*2*-styrylpyridine.
Phenylethyl-*2*-pyridine.
*alpha*-Phenylethyl pyridine.



$C_{13}H_{13}N = 183.26$

Pale yellowish liquid. Almost insoluble in water, soluble in alcohol and oils. B.P. 292° C.

This chemical was developed in a series of experiments aimed at producing pleasant smelling Alkyl- and Aryl-derivatives of Pyridine. Some of these derivatives have found a place in perfumery, but most of them are rare and not commercially available. This is one of the comparatively rare derivatives.

The odor is generally described as "floral, heavy, sweet and tenacious", but there seems to be some difficulty in obtaining samples of identical odor from various suppliers.

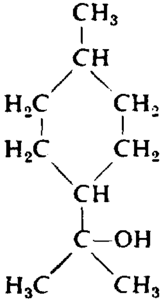
Prod.: from Phenylethyl chloride by heating it with Pyridine in the presence of a Copper catalyst.

(See also 69-525).

See also: Benzyl pyridine.

## 970: DIHYDRO-alpha-TERPINEOL

*para*-Menthan-*8*-ol.
*1*-Methyl-*4*-*iso*-propylcyclohexanol-*8*.
Dimethyl-(*4*-methylcyclohexyl)-carbinol.
(An isomer of Menthol).
*cis*- and *trans*-forms exist.
*trans*-isomer represents the preferred odor (most floral).



$C_{10}H_{20}O = 156.27$

*trans*-Dihydro-*alpha*-terpineol: Needle-like crystals. M.P. 35° C. B.P. 210° C. Sp.Gr. 0.90 (liquid).

Pleasant, floral, Lilac-type odor, softer, yet richer than Terpineol, not quite as lasting. Usually free from undesirable Pine-like notes.

(The *cis*-isomer is more Pine-like, heavier).

Finds some use in perfumery as a modifier for Terpineol in Lilac, Appleblossom, Hyacinth and many other floral fragrances, particularly for low-cost household fragrances, also in New Mown Hay, Fougère, etc. for soaps and detergents.

Prod.:

1) by hydrogenation of *alpha*-Terpineol with Platinum catalyst (this leads to a fairly pure *trans*-Dihydroterpineol).
2) by heating Menthol and Terpineol with a catalyst (this produces Menthone as a by-product).

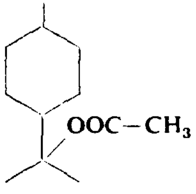
Note: Commercial products will contain some Dihydro-*beta*-terpineol, according to the purity of the starting material.

67-519; 88-52; 156-333; 156-369;

## 971: DIHYDRO TERPINYLACETATE

Dihydro-*alpha*-terpinylacetate.
*para*-Menthan-*8*-yl acetate.
"Menthanyl acetate" (Givaudan).

The commercial product is a mixture of several isomers, including the *cis*-, *trans*-, *alpha*-, and *beta*-forms, mainly *trans-alpha*-Dihydro terpinyl acetate, with considerable amounts of: *trans-beta*-Dihydro terpinyl acetate.



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid, almost insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.94.

Fresh-piney, citrusy and somewhat herbaceous odor. Sweeter and fruitier than Terpinyl acetate, the Dihydro terpinylacetate seems to be cool and warm at the same time (minty-camphoraceous, herbaceous). Its tenacity is not very outstanding.

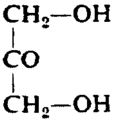
This ester is used quite widely in perfumery, particularly in low-cost Lavender, Citrus, Fougères, etc. for detergents and other household products, and in lower cost Colognes, room-sprays, etc. It constitutes an excellent blender for Linalylacetate, Dihydromyrcenol, Isobornylacetate and many other fresh-piney-fruity or citrusy base chemicals.

Prod.: by hydrogenation of Terpinyl acetate – or by acetylation of Dihydro terpineol.

106-230; 156-369;

## 972: DIHYDROXY ACETONE

"Oxantin".
*1*,*3*-Dihydroxypropan-*2*-one.



$$\begin{array}{l} CH_2-OH \\ | \\ CO \\ | \\ CH_2-OH \end{array}$$

$C_3H_6O_3 = 90.08$

Crystalline white powder. M.P. 72° C. Forms easily a dimer, which melts at 75 to 80° C.

50% soluble in water, 7% soluble in alcohol, poorly soluble in perfume oils and terpenes.

Sweet, cooling taste. Stains the human skin tan, later yellowish. In this respect it resembles Hydroxymethyl furfural. Oxidizes easily in air.

Not a perfume chemical, this material is briefly mentioned because it occurs in cosmetic preparations and influences the odor of the added fragrance significantly. It also has a taste. It is mainly used as a skin-tanning agent.

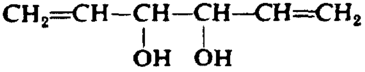
Prod.:

1) from Glycerol by oxidizing action of bacteriae under aerobic conditions.
2) by oxidation of Glycerol by Bromine and Sodium carbonate.

26-504; 66-1039; 100-363; B-I-846;

## 973: 3,4-DIHYDROXY-1,5-HEXADIENE

*1*,*5*-Hexadiene-*3*,*4*-diol.
"Diallylglycol".



$$CH_2{=}CH-\underset{OH}{\underset{|}{CH}}-\underset{OH}{\underset{|}{CH}}-CH{=}CH_2$$

$C_6H_{10}O_2 = 114.15$

Colorless liquid. B.P. 198°C. Sp.Gr. 1.00. Solidifies in the cold, melts at 14°C. or 18°C. (two forms are known).

Soluble in water, miscible with alcohol and most oils.

Faint, musty-vinous odor. Bitter taste, unless very highly diluted. A faint, sweet taste is perceptible at concentrations lower than 40 ppm.

The title material has found a little use in perfume compositions, mainly as a blender, solvent, and for its specific gravity, being almost identical to that of water. Overall for technical purposes more than for olfactory.

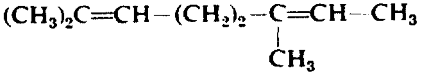
Prod.: by pinacolic reduction of Acrolein.

66-663;

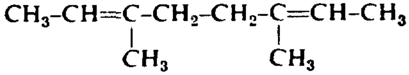
## 974: DI ISOPRENE

The commercial product is normally a mixture of:

1) *2,6*-Dimethyl-*2,6*-octadiene.
2) *2,7*-Dimethyl-*2,6*-octadiene.
3) *3,6*-Dimethyl-*2,6*-octadiene.

1)

$(CH_3)_2C{=}CH-(CH_2)_2-\underset{CH_3}{\underset{|}{C}}{=}CH-CH_3$

2) $(CH_3)_2C{=}CH-(CH_2)_2-CH{=}C(CH_3)_2$

3)

$CH_3\text{-}CH{=}\underset{CH_3}{\underset{|}{C}}\text{-}CH_2\text{-}CH_2\text{-}\underset{CH_3}{\underset{|}{C}}{=}CH\text{-}CH_3$

$C_{10}H_{18} = 138.25$

Colorless, mobile liquid. Insoluble in water, soluble in alcohol and oils.

Sweet, diffusive, somewhat "gassy" odor.

Has been suggested for use in masking odors for industrial purposes. Could possibly find small use in Styrax compositions, etc.

Overall of very little interest to the perfumer.

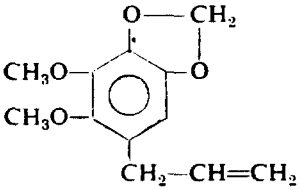
Prod.: by dimerization of Isoprene, using Hydrogen for hydrogen addition in presence of Potassium and Ethyl alcohol.

67-399;

## 975: DILL APIOLE

*1,2*-Methylene dioxy-*4*-allyl-*5,6*-dimethoxybenzene.

An isomer of Parsley-apiole.



$C_{12}H_{14}O_4 = 222.24$

Viscous, almost colorless liquid. B.P. 285° C.

Practically insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Very faint, warm-woody odor. The effect is, however, quite perceptible when this material is used in combination with lower boiling fragrance materials.

Very rarely used in perfumes.

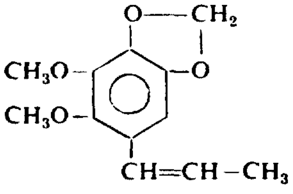
Probably not used in flavors.

Prod.: from East Indian Dill seed oil by isolation. Or: synthetically from Gallacetophenone dimethylether.

65-539; 72-92; 90-487;

## 976: DILL-iso-APIOLE

*1,2*-Methylenedioxy-*4*-propenyl-*5,6*-dimethoxybenzene.



$C_{12}H_{14}O_4 = 222.24$

White or colorless crystals. M.P. 44° C.
B.P. 296° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, warm-camphoraceous and woody odor. When compared to Dill-apiole, it is more camphoraceous than that.

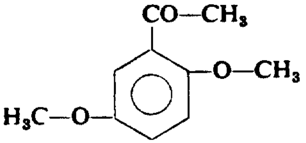
This chemical finds very little use in perfumery, perhaps no use at all in flavors, but it may be a component of certain artificial essential oils and herbal-spicy extracts.

Prod.: by isomerization of Dill apiole with alcoholic alkali.

72-93; 90-488;

## 977: 2,5-DIMETHOXY ACETOPHENONE

*2*-Acetyl dimethylhydroquinone.



$C_{10}H_{12}O_3 = 180.21$

Almost colorless or pale amber-colored oily liquid.

Sweet and faintly Bitter-almond-like balsamic odor of good tenacity.

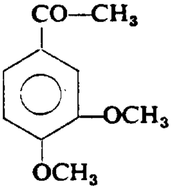
This chemical has found some use in perfume compositions as a part of inexpensive Ambre-bases, particularly in conjunction with Labdanum products with which it blends excellently.

Prod.: from Hydroquinone dimethylether and Acetic anhydride with Aluminum chloride catalyst.

68-754;
(sample: Benzol Products Chemical Co., U.S.A.).

## 978: 3,4-DIMETHOXY ACETOPHENONE

*4*-Acetyl veratrole.
"Acetoveratrone" (misleading name).



$C_{10}H_{12}O_3 = 180.21$

White crystals. M.P. 52° C. B.P. 288° C.

Soluble in hot water, alcohol and oils. Slightly soluble in cold water.

Sweet-woody, very tenacious odor with a pleasant, floral undertone.

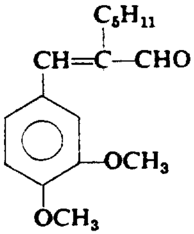
This material could find a little use in perfumery as a component of artificial Orris, Cassie, Mimosa and other bases. However, to the author's knowledge, it is very rarely – if ever, used.

Prod.:

1) by methylation of Acetovanillone.
2) from Veratraldehyde with Acetylchloride and Aluminium chloride.

12-45; 68-753; 86-2; 86-46; 90-540;

## 979: 3,4-DIMETHOXY-alpha-AMYLCINNAMIC ALDEHYDE



$C_{16}H_{22}O_3 = 262.35$

Pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils.

Very faint, sweet-herbaceous odor with a nutlike, oily-sweet undertone.

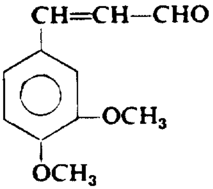
This chemical was developed in an attempt to find substituted Amylcinnamic aldehydes of interest or unique character. However, it has very little to offer, beyond being a fairly good blender-fixative. Its price is too high for that purpose.

Prod.: from *3,4*-Dimethoxybenzaldehyde (Veratraldehyde) by condensation with Heptaldehyde under alkaline conditions.

5-144; 86-46;

## 980: 3,4-DIMETHOXY CINNAMIC ALDEHYDE

Homoconiferaldehyde.
Dimethyl caffeic aldehyde.
Methyl ferulaldehyde.



$C_{11}H_{12}O_3 = 192.22$

Yellowish oily liquid. Very slightly soluble in water, soluble in alcohol and oils.

Warm-spicy, sweet, almost balsamic-woody odor with rich, sweet and slightly nutlike, long lasting undertones.

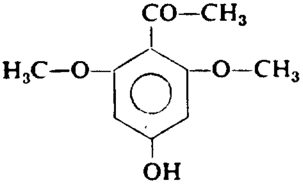
This aldehyde has been suggested for use in flavor compositions as a modifier for Coniferaldehyde (very rarely available), mainly in Maple flavors, Nut compositions, Caramel, Vanilla, etc.

To the author's knowledge, it has not found much use in perfumery.

Prod.: by condensation of Veratraldehyde with Acetaldehyde (Claisen condensation).

## 981: 2,6-DIMETHOXY-4-OXYACETOPHENONE

*2,6*-Phloracetophenone dimethylether.
*3,5*-Dimethoxy-*4*-acetylphenol.
*iso*-Xanthoxylin.*)



$C_{10}H_{12}O_4 = 196.21$

Colorless or white crystals. Almost insoluble in water, soluble in alcohol and oils.

Sweet-balsamic, slightly animal and heavy odor of good tenacity.

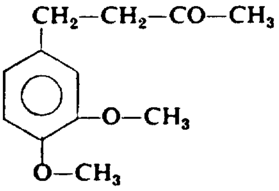
This material has been suggested for use in perfume compositions where it has shown to be of effect in heavy balsamic type fragrances, particularly in conjunction with Labdanum, Castoreum, Vanilla, Oakmoss, etc.

It is less stable than Dimethoxy acetophenone, but it is also softer and mellower of odor.

*) Xanthoxylin, a naturally occurring material is:
*2,4*-Dimethoxy-*6*-hydroxy acetophenone, or
*2,4*-Phloracetophenone dimethylether.

## 982: 3,4-DIMETHOXY PHENYLETHYL METHYLKETONE

*1*-(*3,4*-Dimethoxyphenyl)-*3*-butanone.
*3,4*-Dimethoxy benzylacetone.
"Methyl zingerone".



$C_{12}H_{16}O_3 = 208.26$

Colorless or white needle-like crystals.
M.P. 56° C. B.P. 287° C.

Insoluble in water, soluble in alcohol and oils.

Sweet and warm-floral odor of balsamic-Vanilla-like character and excellent tenacity.

This rare material (rarely offered under its proper chemical name) finds some use in perfume compositions as a fixative/blender with Tolu balsam, Perubalsam, heavy floral materials, Castoreum, etc. for balsamic and sweet or powdery background notes.

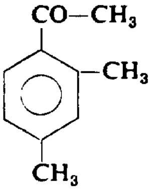
It does not discolor under daylight or in presence of iron, but it does not yield the same amount of sweetness as Vanillin. On the other hand, it is richer in balsamic effect, and quite versatile since it does not override a fragrance with an easily recognizable note (such as Vanillin may often do it).

Prod.:

1) from Acetone and Veratraldehyde, followed by hydrogenation.
2) by careful Methylation of Zingerone (see monograph) which is obtained from Vanillin and Acetone condensation, followed by hydrogenation. The product is subsequently methylated.

## 983: 2,4-DIMETHYL ACETOPHENONE

Acetyl-*meta*-xylene.
Commercial product is a mixture of *meta*- and *para*-isomers.



$C_{10}H_{12}O = 148.21$

Colorless liquid. Sp.Gr. 1.01. B.P. 228° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral, woody odor, rather pungent in the pure state, but almost Mimosa-like in extreme dilution or in proper composition with other perfume chemicals.

Used in perfume compositions for New Mown Hay, Fougère, Clover, Mimosa and other floral and non-floral perfumes, mainly in soap and detergent perfumes, room sprays, etc.

Finds a little use in flavor compositions for imitation Grape, in Vanilla flavors, Cream-soda compositions, etc.

Concentration is normally mere traces.

Prod.:

1) as a by-product in the manufacture of Musk Ketone.
2) from *meta*-Xylene and Acetyl chloride.

G.R.A.S. F.E.M.A. No.2387.

4-45; 68-96; 68-532; 86-46;

## 984: DIMETHYL ACROLEIN

*beta*-Methylcrotonaldehyde
*beta*-*beta*-Dimethyl acrolein.
*3*-Methylbuten-*2*-al-*1*.
An isomer of Tiglic aldehyde.

$(CH_3)_2C{=}CH{-}CHO$

$C_5H_8O = 84.12$

Colorless mobile liquid. B.P. 135° C.
Sp.Gr. 0.87.

Almost insoluble in water, soluble in alcohol and oils.

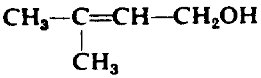
Powerful and very diffusive, penetrating "gassy" odor of green-ethereal character. Very poor tenacity.

This aldehyde has found use in flavor compositions, mainly in the reconstitutiion of Raspberry flavor and "true-to-Nature" mitation Raspberry. It is used in trace concentrations only, but lends a powerful lift of freshly pressed juice to the aroma.

159-666; 66-503;

## 985: beta-beta-**DIMETHYL ALLYLALCOHOL**

*3*-Methylbuten-*2*-ol-*1*.
*3*-Methyl crotyl alcohol.



$$CH_3{-}\underset{\displaystyle CH_3}{\underset{|}{C}}{=}CH{-}CH_2OH$$

$C_5H_{10}O = 86.14$

Colorless mobile liquid.

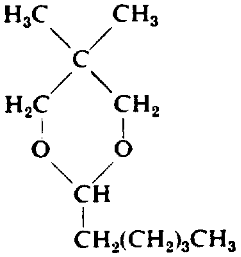
Sharp, green-oily, somewhat "gassy" odor. When properly diluted, it displays rather pleasant, winey-fermentation-like notes.

The taste is – in high dilution – winey-Brandy-like, somewhat green.

This alcohol has been developed for the purpose of making more "true-to-Nature" Raspberry flavors, but it is only a minor component and it is a rare chemical on the market.

## 986: 5,5-**DIMETHYL**-2-n-**AMYL**-1,3-**DIOXANE**

Hexaldehyde-*2,2*-dimethyl-*1,3*-propanediol, cyclic acetal.



$C_{11}H_{22}O_2 = 186.30$

Colorless, slightly viscous liquid.

Slightly soluble in water, soluble in alcohol and oils.

Powerful and relatively diffusive, fruity-floral odor of Pineapple-Jasmin character. The fruity notes are refreshingly green, without being sharp, the floral notes are intense and sweet, yet very fresh and lively.

The title cyclic acetal represents a series of products, developed from a Glycol, different from the conventional and ordinarily available Glycols. The condensation products from Aldehydes and ketones with this Glycol have been prepared in great number and variety, and some of the materials have been very interesting. The title material may have some potential interest to the modern creative perfumer. It is readily prepared, if not commercially available, it is inexpensive and stable in all conventional perfume materials and functional products, and it has a very versatile fragrance type.

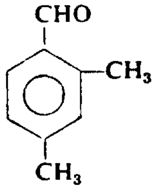
Prod.: from Hexaldehyde by condensation with *2,2*-Dimethyl-*1,3*-propanediol.

The condensation product with Heptaldehyde is also known. It has a more nut-like, Jasmin-Melon-like herbaceous-floral character.

See also: *2,5,5*-Trimethyl-*2*-amyl-*1,3*-dioxane. Perfumery and Essential Oil Record, July 1966, pages 427-433;

## 987: 2,4-**DIMETHYL BENZALDEHYDE**

*2,4*-Xylylaldehyde.



$C_9H_{10}O = 134.18$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 216° C.

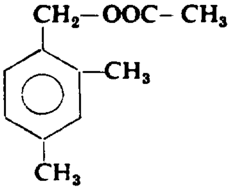
Mild "Bitter-Almond" type odor, weaker and sweeter than that of Benzaldehyde, somewhat floral and more stable towards oxidation.

Has been suggested for use in perfume compositions, where Benzaldehyde is undesirable on account of its poor stability. It remains, however, a comparatively rare chemical, and it still finds competition in the much less expensive Benzaldehyde.

Prod.: by Manganese peroxide oxidation of *1,2,4*-Trimethyl benzene (Pseudo-cumene).

68-107; 86-47; 68-515;

## 988: 2,4-DIMETHYL BENZYL ACETATE



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-floral, rather fresh and somewhat fruity odor of moderate tenacity.

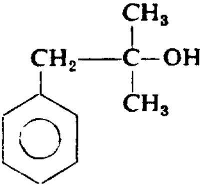
Has been suggested for use in perfume compositions, mainly as a modifier for Benzyl acetate in Jasmin bases, where better tenacity is desirable. Also in general as a floral-fruity body for partial substitution of Benzyl acetate, or as a modifier for the so-called Tolyl acetate (Methyl benzyl acetate).

This chemical is used but not commonly available from the regular suppliers of perfume chemicals.

Prod.: from *2,4*-Dimethylbenzylalcohol, which can be obtained by reduction of the aldehyde (see previous monograph).

## 989: DIMETHYL BENZYL CARBINOL

D.M.B.C.
Benzyl dimethyl carbinol.
"Surolene" (old French trade name).
*alpha-alpha*-Dimethyl phenyethylalcohol.
*beta*-Hydroxy-*beta*-benzylpropane.
Phenyl-*tertiary*-butylalcohol.
*alpha*-Benzyl-*iso*-propylalcohol.



$C_{10}H_{14}O = 150.22$

White or translucent crystalline mass, melting at 24° C. B.P. 215° C. Sp.Gr. (liquid) 0.98.

The liquid is a colorless viscous oil, very slightly soluble in water, soluble in alcohol and oils, also in Propylene glycol, but not in Glycerin.

Warm-herbaceous-floral, slightly animal odor, reminiscent of Lilac and Elderflowers with undertones of fresh cut wood.

Excellent perfume material for Lilac, Narcissus, Jasmin, Muguet, Hyacinth, Mimosa, Neroli, and in certain types of Rose (Safran-like notes). It is stable in soap and blends excellently with its homologues, esters and with a great number of other perfume chemicals.

Finds some use in flavor compositions, mainly for imitation Coffee, Rhubarb, Pear, Gooseberry, Blackcurrant, Green Pepper, etc.

Normal concentration in the consumer product is but a few ppm, while it may be as high as 100 ppm in chewing gum.

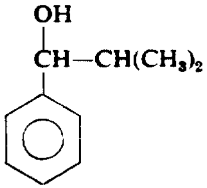
FCC-1964-813; G.R.A.S.
F.E.M.A. No.2393.

Prod.: by Grignard synthesis from Benzylmagnesium chloride and Acetone.

4-45; 5-66; 34-161; 36-815; 37-513; 86-47; 106-136; 156-76;

## 990: iso-DIMETHYL BENZYL CARBINOL

*alpha-iso*-Propyl benzylalcohol.
*alpha-alpha*-Dimethyl-*beta*-hydroxyphenyl ethylene.
"*iso*-D.M.B.C.".
*iso*-Propyl phenylcarbinol.
Phenyl-*iso*-propylcarbinol.



$C_{10}H_{14}O = 150.22$

Colorless, somewhat viscous liquid.
B.P. 224° C. Sp.Gr. 0.99.

Warm, woody-rosy odor of moderate to good tenacity. When used with sweeter materials, it produces very pleasant, rich, mellow rose notes and "depth" of warm undertones.

This "carbinol" has been suggested for use in perfume compositions and finds limited use in such, although not parallel to the isomer, Dimethylbenzylcarbinol. The title material is more rosy-woody, and less green. It may be slightly more difficult to employ, but with proper blending it can yield satisfactory results and justify further use of this material.

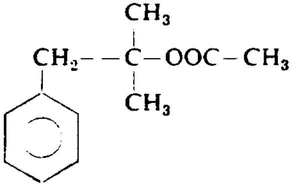
It is rarely offered under its proper chemical name, but often manufactured by the specialists in making the "perfumery carbinols".

Prod.: by Grignard reaction from Benzaldehyde and *iso*-Propyl magnesiumbromide. It has also been prepared by reduction of *iso*-Propylphenylketone.

68-501; see also: 36-815;

## 991: DIMETHYL BENZYL CARBINYL ACETATE

D.M.B.C.A.
Benzyldimethyl carbinylacetate.
Benzyl-*iso*-propylacetate.
*alpha-alpha*-Dimethyl phenylethylacetate.



$C_{12}H_{16}O_2 = 192.26$

White or colorless crystals. M.P. 30° C. – or colorless liquid. Sp.Gr. 1.00 (0.99 liquid). B.P. 250° C.

Soluble in alcohol, perfume oils and mineral oil, poorly soluble in Propylene glycol, insoluble in Glycerin.

Fresh and powerful, floral-fruity, slightly herbaceous odor of Jasmin-Lily type. The commercial product may contain 1-2% Benzylacetate which influences the topnote character, but otherwise is harmless to the general use of this chemical.

Widely used in perfume compositions, mainly for better soap perfumes, cosmetic fragrances. It is commonly used in Jasmin bases, Rose, Muguet, Geranium, Hyacinth and other florals, as well as Chypre types. It blends well with the parent alcohol and with homologue esters, with *para-tertiary*-Butyl cyclohexylacetate and similar chemicals.

Finds some use in flavor compositions for imitation Cherry and Honey, since its flavor resembles that of Beeswax – in proper dilution. It has also been used in Rhubarb and Green Peppers type of flavor compositions.

The concentration in candy is normally about 20 ppm.

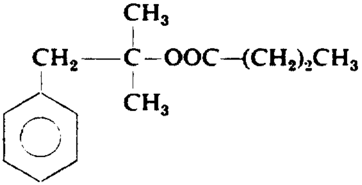
Prod.: by direct esterification, using a catalyst at low heat.

FCC-1964-815; G.R.A.S.
F.E.M.A. No.2392.

5-66; 4-45; 33-501; 77-184; 86-47; 106-137; 156-76;

## 992: DIMETHYL BENZYL CARBINYL BUTYRATE

D.M.B.C. butyrate.
Benzyl dimethylcarbinyl-*n*-butyrate.
*alpha-alpha*-Dimethyl phenylethyl butyrate.



$C_{14}H_{20}O_2 = 220.31$

Colorless, slightly oily liquid. Insoluble in water, soluble in alcohol and oils.

Mild-herbaceous, fruity odor in the Plum/Prune type. The undertones in a good-quality, acid-free ester are extremely pleasant, tea-like, warm and sweet. Needless to add, that the smallest traces of free Butyric acid are quite detrimental to this odor picture.

Used in perfume compositions of the Oriental-Rose, Chypre, Peony and other types, often as a modifier for other D.M.B.C. esters.

Finds some use in fruit flavors, particularly in Apricot, Peach, Plum, Prune and European type of Cherry (non-almondy).

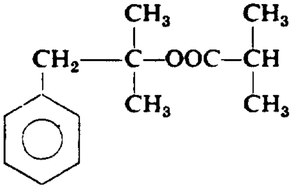
The concentration in food or candy will normally be about 20 ppm.

G.R.A.S. F.E.M.A. No.2394.

Prod.: by direct esterification of Dimethyl benzylcarbinol with *n*-Butyric acid, using a catalyst and preferably azeotropic conditions.

## 993: DIMETHYL BENZYL CARBINYL-iso-BUTYRATE

D.M.B.C.-*iso*-butyrate.
*alpha-alpha*-Dimethylphenylethyl-*iso*-butyrate.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

The odor is slightly fresher (less "heavy") than that of the *n*-Butyrate, less warm, more "chemical", but also more stable than the normal ester.

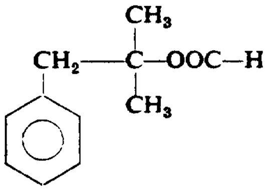
Finds some use in perfumery as a modifier-blender in Lavender compositions, Rose, Chypre types and floral fragrances. It has good tenacity and blends well with herbaceous as well as floral materials.

Occasionally used in flavor compositions. It is NOT listed in the G.R.A.S. list of the U.S. Federal Register, but it is conceivable that the acceptance of the normal ester could cover the subject material, too.

Prod.: by direct esterification of D.M.B.C. with *iso*-Butyric acid in presence of a catalyst and preferably under azeotropic conditions.

## 994: DIMETHYL BENZYL CARBINYL FORMATE

*alpha-alpha*-Dimethyl phenylethyl formate.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid, almost insoluble in water, soluble in alcohol and oils.

Dry, herbaceous-green, Narcissus-Lily-Jasmin type of odor. Rather pungent in its green notes, but not unpleasant.

Although very rarely offered commercially, this chemical is used – mainly by a few producers – in perfume compositions of the named types, also in Hyacinth, Ambre, etc.

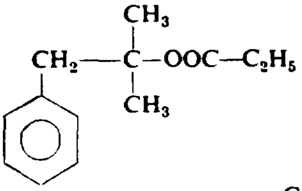
Traces of this chemical are used in various types of Spice flavor compositions, where its warm-herbaceous flavor can give quite unique effects.

G.R.A.S. F.E.M.A. No.2395.

Prod.: directly from D.M.B.C. and Formic acid, usually with the aid of Acetic anhydride.

## 995: DIMETHYL BENZYL CARBINYL PROPIONATE

Benzyl-*iso*-propyl propionate.
D.M.B.C. propionate.



$C_{13}H_{18}O_2 = 206.29$

Colorless, slightly oily liquid. Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Sweet-floral, fruity odor of good tenacity.

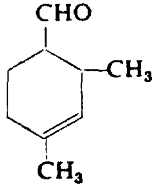
The fact that the odor of this ester is rather nondescript, not typically fruity, not clearly floral, and not reminiscent of one distinct natural product, has probably produced some difficulty in the extended use of D.M.B.C. propionate.

It finds some use in perfumery for the more delicate and fruity floral types, such as Freesia, Sweet Pea, Peony, Magnolia, occasionally also as a modifier in Jasmin, Narcissus, etc. and in various fantasy fragrances.

Prod.: by direct esterification of D.M.B.C. with Propionic acid or Propionic anhydride.

## 996: 2,4-DIMETHYL BUTADIENEACROLEIN

The material offered under the title name is:
*2,4*-Dimethyl tetrahydrobenzaldehyde.
*2,4*-Dimethylcyclohex-*3*-enealdehyde.



$C_9H_{14}O = 138.21$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Moderately powerful, sweet-green, leafy odor of mediocre tenacity.

This aldehyde has, among several isomers and homologues, found some use in perfume compositions, mainly as part of new topnote compositions, specialties and bases.

It performs very well with Galbanum and Citrus oils, and it is compatible with floral, woody and herbaceous notes.

The material is rarely offered under its proper chemical name, although it was developed in an extensive research program by a large chemical company, not in the perfume chemical business, many years ago.

Interesting derivatives of potential use in perfume compositions have been prepared from this aldehyde (and its isomers and homologues) by condensation with Acetone, a process analogous to the Ionone synthesis. Many of the resulting Tetrahydrobenzylidene acetones are used in perfumes.

See also monograph: *3,4*-Dimethyl tetrahydrobenzaldehyde.

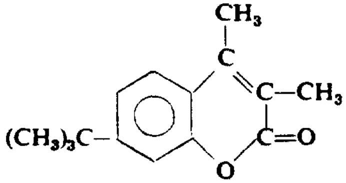
Prod.: from Butadiene and Tiglic aldehyde.

Also from Dimethyl butadiene and Acrolein.

67-190;

## 997: 3,4-DIMETHYL-7-tertiary-BUTYL COUMARIN

"Butolia".
"Lychenone".
*tertiary*-Butyl dimethylcoumarin.



$C_{15}H_{18}O_2 = 230.31$

White or very pale ivory-colored or cream-colored crystals. Almost insoluble in water and Propylene glycol. Poorly soluble in cold alcohol, soluble in hot alcohol. Soluble in most perfume oils.

Sweet, musky and nut-like, Hazelnut-Coconut type odor with discrete animal undertones, resembling certain notes in Musk, Civet and Castoreum, pleasantly free from any trace of faecal notes.

In actual use, incorporated in a perfume, it introduces a delicate, sweet-leathery note, less animal than the note achieved with Castoreum, and quite similar to the odor of Russian (cured) leather.

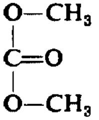
This Lactone performs very well with Oakmoss products, Juniperberry oil (deterpenized), Clary Sage absolute, Clove products, etc. and with the sweet and heavy wood notes in Chypre, "Miss Dior" types, etc. It is also of interesting effect in Men's fragrances, leathery or non-leathery types. The effect of this material resembles to a certain degree that of 7-Methyl coumarin, the latter being less leathery, however.

Prod.: from Diketen.

(Samples: Norda Ess. Oil & Chem. Co. - and Agfa, Chem. Fabr.).

## 998: DIMETHYL CARBONATE

Methylcarbonate.



$$\begin{array}{l} O-CH_3 \\ | \\ C{=}O \\ | \\ O-CH_3 \end{array}$$

$C_3H_6O_3 = 90.08$

Colorless liquid. B.P. 90° C. Sp.Gr. 1.06.

Solidifies in the cold, melts again at ÷0.5° C.

Insoluble in water, soluble in alcohol and oils.

Very diffusive, ethereal odor of poor tenacity. The sweetness resembles that of Acetone, but is not nearly as choking.

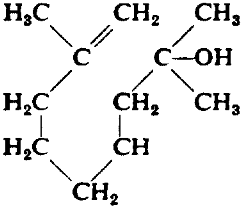
This relatively unusual ester has found a little use in perfumery as part of certain top-note compositions, where it enhances the radiation or "diffusive power" by its high vapor pressure and relatively neutral odor type, blending well with the Citrus oils and herbaceous oils, even with many floral compositions. In alcoholic solutions, including "colognes", it may assist in distracting from the odor of alcohol, being a material of almost the same boiling point, it has good "masking" property for such purpose.

Prod.:

1) from Chloroformic ester by heating with lead oxide.
2) from Carbonyl chloride (Phosgen) with Methanol.

26-516; 66-888; 100-673; B-III-4;

## 999: DIMETHYL CITRONELLOL



$C_{12}H_{24}O = 184.32$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Somewhat dry, camphoraceous-rosy odor, vaguely reminiscent of the odor of Citronellol.

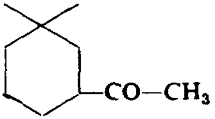
This material - an isomer of "Ethylcitronellol" (see later) - is of very little interest to the perfumer.

Prod.: from Citronellol.

31-17;

## 1000: 1,1-DIMETHYL CYCLOHEX-3-ENYL METHYLKETONE

*3*-Acetyl-*1*,*1*-dimethyl-*3*-cyclohexene.



$C_{10}H_{16}O = 152.24$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, herbaceous, somewhat weedy, but basically sweet odor of moderate tenacity.

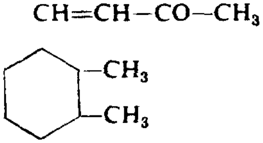
This chemical, rarely offered as such, but frequently used in the state of a component of certain perfume material specialties, finds use in soap perfumes and a few types of detergent perfumes, etc. Its power and stability, its "lifting" effect upon Lavender, Rose, Fougères, etc. are its greatest assets.

Prod.: This ketone occurs as a minor component in the reaction mixture from treatment of Myrcene hydrochloride with acetylating agents via various methods.

The Myrcene is obtained from *beta*-Pinene by pyrolysis, and the reaction product is treated with hydrogen chloride to yield Myrcene hydrochloride.

The acetylation process is an offspring of the patented, but not much used, process of preparing Linalyl acetate directly from Myrcene.

## 1001: 1-(2,3-DIMETHYLCYCLOHEXYL)-1-BUTEN-3-ONE



$C_{12}H_{20}O = 180.29$

Almost colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

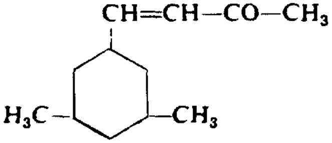
Sweet, fruity-woody odor of moderate tenacity. The fruity notes are rather ethereal or winey, while the woody notes are sweet and remotely resembling those of *alpha*-Ionone, yet not as powerful.

This ketone has been suggested for use in perfume compositions, and it was developed in the course of a research program aimed at new odor chemicals from Acetone condensation with alifatic or alicyclic aldehydes.

The material is very rarely offered under its proper chemical name, and it has not succeeded in catching the interest of many perfumers. It will most likely remain an article of academic interest only.

Prod.: by condensation of Acetone with *2,3*-Dimethylcyclohexane carboxaldehyde.

## 1002: 1-(3,5-DIMETHYLCYCLOHEXYL)-1-BUTEN-3-ONE



$C_{12}H_{20}O = 180.29$

Almost colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Sweet-fruity-woody odor, but somewhat drier than that of the *2,3*-isomer (see previous monograph). Moderate tenacity and pleasant terminal notes reminiscent of refined, sweet-woody Oakmoss notes. The fruity notes are less pronounced in this isomer.

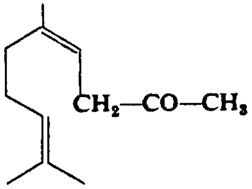
A rare chemical, probably confined to the research shelf, and only occasionally found in the perfume laboratory. Not offered commercially under its proper chemical name.

See also notes under the isomer (previous monograph).

Prod.: by condensation of Acetone with *3,5*-Dimethyl cyclohexancarboxaldehyde.

## 1003: 5,9-DIMETHYL-4,8-DECADIEN-2-ONE

"Citralone" (Givaudan Corp.).



$C_{12}H_{20}O = 180.29$

Pale yellowish oily liquid. **B.P.** 242° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet and lemony odor, not nearly as sharp as Citral, and much more tenacious.

This ketone, for a long time marketed only under a trade name as a popular specialty, has found good use in perfume compositions, where a Lemon-like effect may be desirable, but the presence of a sensitive aldehyde may be a problem.

Although this material is in no way a substitute for Citral, it can offer similar effects, and, in many cases, prove to be more versatile and longer lasting. It is particularly interesting in heavy floral fragrances where Anthranilates may be present, and normally would cause considerable darkening in presence of Citral.

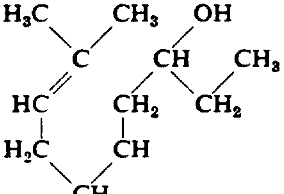
The cyclized product, also a perfume material, and known under the name "Cyclocitralone" is listed in this work under: *5*-Methyl-*2*-*iso*-propyl-*1*-acetyl-*5*-cyclohexene.

Prod.: (title material) from Citral with Ethyl *alpha*-chloropropionate and Sodamide via Citral ethylglycidate by saponification to the glycidic acid which yields the ketone by decarboxylation.

31-97; 163-18;

## 1004: 5,9-DIMETHYL-8-DECEN-3-OL

"Ethyl citronellol" (incorrect name).
("Ethyl geraniol" – incorrect name).



$C_{12}H_{24}O = 184.32$

Colorless or very pale straw-colored oily liquid.

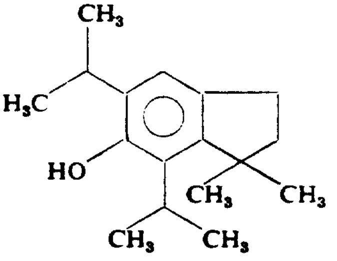
Very slightly soluble in water, soluble in alcohol and oils.

Semi-sweet, oily-rosy odor, more waxy than that of Citronellol, more tenacious, but also somewhat drier.

Finds use in perfumes, mainly for soaps and detergents. It is not commonly available, but mostly used by a few manufacturers of this chemical.

## 1005: 1,1-DIMETHYL-5,7-DI-iso-PROPYL-6-INDANOL

An Indanol type musk by Givaudan Corp. (Future name and full information not available at the time of editing this monograph, Sept. 1968).



$C_{17}H_{26}O = 246.40$

This material, which is not yet commercially available (Sept. 1968) appears to be a very promising new type musk.

It is unusual in being a phenol, and it is reported to have antioxidant properties.

From a production point of view, it is encouraging, since it can be made in a one-step simple reaction from readily available chemicals.

Temporary comments are given in "The Givaudanian", June 1968, page 8.

(Givaudan Corp. patent pending).

## 1006: DIMETHYL DISULFIDE

Methyl disulfide.

$CH_3—S—S—CH_3$

$C_2H_6S_2 = 94.20$

Pale yellowish, mobile liquid. Sp.Gr. 1.06. B.P. 112° C.

Very slightly soluble in water, soluble in alcohol and oils. Intensely onionlike, very diffusive odor. Non-lachrymatory.

Finds use in flavor compositions, almost exclusively those of Onion or Cabbage-type. It serves as part of the flavor for "reconstitution" of natural flavor lost during processing of the consumer product.

Concentration is about 1 to 3 ppm in the finished product.

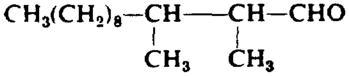
Prod.: from Methyl bromide and Sodium thiosulfate. The resulting Sodium methylthiosulfate is converted by heating to yield Dimethyl disulfide.

NOTE: Do not confuse with Dimethyl sulfide (see this monograph).

26-604; 66-349; 90-824; 105-489; B-I-291; 61-Nov.-53;

## 1007: 10,11-DIMETHYL DODECANAL

"Dimethyl nonyl acetaldehyde" (misleading name).
*alpha-beta*-Dimethyl dodecylaldehyde.
An isomer of Myristic aldehyde.



$CH_3(CH_2)_8-\underset{CH_3}{\underset{|}{CH}}-\underset{CH_3}{\underset{|}{CH}}-CHO$

$C_{14}H_{28}O = 212.38$

Colorless oily liquid, insoluble in water, soluble in alcohol and oils.

Intensely waxy, dry-floral odor, almost typical of the term "aldehydic" and even drier than the odor of Methyl nonyl acetaldehyde.

Has been recommended for use in perfume compositions as a variation of the "MNA"-type topnote in Ambre, Chypre, Citrus and many other fragrance types.

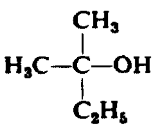
However, it is not commonly available and rarely offered commercially.

Prod.: from Methyl nonyl ketone by condensation with Bromopropionic acid.

31-50;

## 1008: DIMETHYL ETHYL CARBINOL

*tertiary*-Amylalcohol.
*2*-Methylbutanol-*2*.



$H_3C-\overset{\overset{CH_3}{|}}{\underset{\underset{C_2H_5}{|}}{C}}-OH$

$C_5H_{12}O = 88.15$

Colorless liquid. Sp.Gr. 0.81. B.P. 102° C.

Slightly soluble in water, soluble in Propylene glycol, alcohol and oils.

Nauseating, Camphor-like odor, also slightly cool, minty, diffusive.

The vapors of this chemical have a hypnotic effect on the human Central Nervous System.

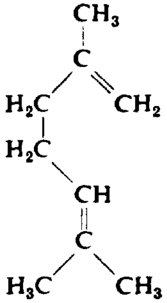
Has been suggested for use in masking odors for technical/industrial purposes, but since this chemical is more toxic than *iso*-Amylalcohol (ordinary Amylalcohol), it has by and large been abandoned as a fragrance material.

Prod.: from Trimethyl ethylene plus Sulfuric acid.

26-406; 66-312; B-I-388;

## 1009: 2,6-DIMETHYL-2,6-HEPTADIENE

Geraniolene.



$C_9H_{16} = 124.23$

Colorless liquid. Turns yellowish or straw-colored when exposed to air and daylight. B.P. 284° C. Sp.Gr. 0.77.

Insoluble in water, soluble in alcohol, miscible with most oils.

Sweet, somewhat woody-rosy odor with resemblance to the odor of distilled tail fractions from Geraniol, yet not as tenacious.

Has been suggested for use in perfume compositions. However, only if this chemical could be made available at very low cost, it would have a chance of survival among the many low-cost by-products from Geraniol (synthetic and natural) now available.

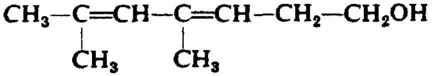
It could also find some use in artificial essential oils.

Prod.: from Geranic acid by heating (decarboxylation).
Also from *2,6*-Dibromo-*2,5*-dimethylheptane.

66-645; 86-54; 87-557

## 1010: 4,6-DIMETHYLHEPTADIEN-(3,5)-OL-(1)

An isomer of "Violet leaf alcohol" (see *2,6*-Nonadienol).



$$CH_3-\underset{CH_3}{C}=CH-\underset{CH_3}{C}=CH-CH_2-CH_2OH$$

$C_9H_{16}O = 140.23$

Colorless or pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

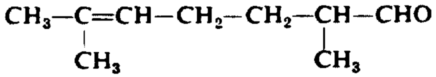
Oily-green, powerful and sweet odor. Less Cucumber-like and more floral than the "Violet leaf alcohol", also sweeter.

This is a very rare chemical, not offered commercially from the conventional manufacturers of perfume chemicals.

It has been suggested for use in perfume compositions as a topnote-ingredient in delicate floral fragrances (Muguet, etc.) and in Citrus compositions. It imparts very fresh and pleasant notes to Bergamot oil, Lavender etc.

## 1011: 2,6-DIMETHYL-2-HEPTENAL-(7)

*2,6*-Dimethyl-*5*-hepten-*1*-al.
*2,6*-Dimethyl heptaldehyde.
"Melonal" (Givaudan).



$$CH_3-\underset{CH_3}{C}=CH-CH_2-CH_2-\underset{CH_3}{CH}-CHO$$

$C_9H_{16}O = 140.23$

Pale yellowish oily liquid. Color and viscosity increases upon storage (polymerization and oxidation). Sp.Gr. 0.84.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Very powerful, oily-green, vegetable-like odor, reminiscent of Melon-skins (outer peel of Melon). In extreme dilution sweeter, more typical Melon-like, refreshing.

This aldehyde finds some use in perfume compositions, partly as a modifier for the common alifatic aldehydes in fresh, outdoorish and clean odors, partly as a masking agent for various purposes. It is a common ingredient in fragrances for the type of handlotion known ad "Cucumber-lotion".

It is also used sparingly in various fruit flavors, vegetable flavors, etc. Concentration in the finished product is usually from 1 to 20 ppm.

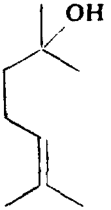
G.R.A.S. F.E.M.A. No.2389.

Prod.: by condensation of *iso*-Butyric aldehyde with *beta*-Methylcrotonaldehyde, followed by partial hydrogenation.

31-39; 41-192; 106-229;

## 1012: DIMETHYL HEPTENOL

*2,6*-Dimethyl-*2*-hepten-*6*-ol.
"Brazinol" (Rhodia, Inc.).
*2,6*-Dimethyl-*5*-heptenol (F.D.A.-name).



$C_9H_{18}O = 142.24$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet and refreshing floral odor with discretely woody-herbaceous or mildly balsamic notes. Very suggestive of Lavender/Clary Sage.

This alcohol, developed in the research projects leading to new processes for the manufacture of Lavandulol, has been marketed as a "Bois de Rose" chemical a few years ago. It was at the time of very poor supply and very high market prices of Lavandin oil, but the initial price of the title material was prohibitive for its use in Lavandin substitute.

The material has followed the trend of many other aromatic chemicals on their way to possible success: A few years of very slow sales, reluctance from the perfumers, and objection to the high cost. Eventually, the material became available at a price which allowed for rather free use of it in perfume formulations, in soap perfumes, and in artificial essential oils. It is in competition with Linalool with respect to cost.

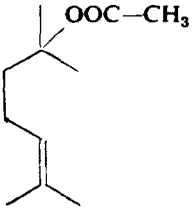
The title alcohol has the pungent power of Spike Lavender, the floral character of Linalool, and the sweet-balsamic tonalities of Tetrahydromuguol, e. g. Which makes it a very versatile material, useful in Lime, Lavandin, Muguet, Lilac, Rose, woody and balsamic types, etc.

It blends very pleasantly with Oakmoss and Opopanax products.

87-501; 87-576; (Rhodia literature).
NOTE: *2,6*-Dimethyl-*5*-heptenol is G.R.A.S. by F.D.A. (American F.D.A.).

## 1013: DIMETHYL HEPTENYL ACETATE

"Brazinyl acetate" (Rhodia, Inc.).
*2,6*-Dimethyl-*2*-hepten-*6*-yl acetate.



$C_{11}H_{20}O_2 = 184.28$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, herbaceous-spicy, mildly balsamic odor of moderate tenacity. The spicy balsamic notes have some resemblance to Opopanax.

This ester was developed along with the alcohol (see previous monograph) and appeared on the perfumery market at the time of extreme scarcity of Lavandin oil. The title material was not priced favorably at that time, and it may not have harmed this ester very much, because it should be considered as an individual perfume chemical, not as a substitute for Linalylacetate, or a type of that ester.

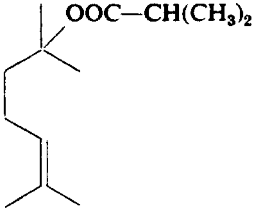
It is considerably more powerful and penetrating, and lends itself to novel creations for soap, etc.

It blends particularly well with the herbaceous oils, Amylsalicylate, Labdanum, Geranium etc. for general cosmetic fragrance creation, and since it does not have the distinctly fruity, Pear-like note of Linalylacetate, but rather a deep-Plum-like fruitiness, it blends better with the Methylionones.

See also: Dimethyl heptenol.

## 1014: DIMETHYL HEPTENYL-iso-BUTYRATE

*2,6*-Dimethyl-*2*-hepten-*6*-yl-*iso*-butyrate.
"Brazinyl-*iso*-butyrate". (Rhodia, Inc.).



$C_{13}H_{24}O_2 = 212.34$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Heavy, fruity-balsamic odor of good tenacity.

This ester has only recently been marketed, and it is probably too early to predict its future in perfumery.

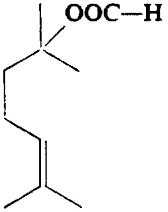
Its peculiar fruity-resinous-balsamic sweetness is quite characteristic of this series of esters, and it makes them suitable for Oriental fragrance creations with Opopanax, Labdanum, Patchouli, etc.

After a few years in use, it will probably be possible to determine whether this material has a permanent place on the perfumer's shelf, or it will fall back into the cabinet of research chemicals, but the first step has been taken by the manufacturer: the material is commercially available.

See also: Dimethyl heptenol.

## 1015: DIMETHYL HEPTENYL FORMATE

*2,6*-Dimethyl-*2*-hepten-*6*-yl formate.
"Brazinyl formate" (Rhodia).



$C_{10}H_{18}O_2 = 170.25$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, citrusy-herbaceous, balsamic-green odor of moderate tenacity.

This ester has recently been marketed among several other esters of Dimethyl heptenol. Although the alcohol was known and available long before this ester became commercially available, there is reason to assume that the alcohol will become more popular than the esters, maybe except the acetate (see previous monograph).

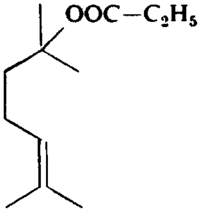
Very few formates are being used in real volume (Citronellyl formate is one of them), and the title ester does not have enough character of its own to justify very optimistic predictions for its future in perfumery.

It performs very well in various types of household fragrance, and gives pleasant effects with Citrus-Lavender types, Citrus-Fougères, etc.

See also: Dimethyl heptenol.

## 1016: DIMETHYL HEPTENYL PROPIONATE

*2,6*-Dimethyl-*2*-hepten-*6*-yl propionate.
"Brazinyl propionate" (Rhodia, Inc.).



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, fruity-balsamic, mildly spicy odor of good tenacity. The balsamic notes have the same resinous sweetness as encountered in the acetate, but the fruity-balsamic character is generally emphasized in this ester.

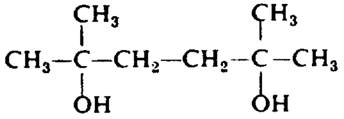
The title ester was made commercially available recently (1968) after the earlier marketing of the alcohol. With the attractive price level and a relatively versatile odor pattern in mind, one can predict some future for these esters, although they cannot compete in price with the *iso*-Dihydro lavandulyl esters, often used for similar purposes.

It is still too early to make firm statements about the success of this ester.

See also: Dimethyl heptenol.

## 1017: DIMETHYL HEXANEDIOL

*2,5*-Dimethyl-*2,5*-hexanediol.



$$CH_3-\underset{OH}{\overset{CH_3}{C}}-CH_2-CH_2-\underset{OH}{\overset{CH_3}{C}}-CH_3$$

$C_8H_{18}O_2 = 146.23$

Colorless or white crystals. M.P. 93° C. B.P. 213° C.

Soluble in water, miscible with alcohol and most oils.

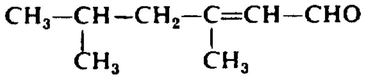
Faint, camphorlike odor.

This material has been used as a solvent in certain fragrance types, but the author believes that the use of subject material is practically abandoned in perfumery and flavors.

Prod.: by hydrogenation of *2,5*-Dimethyl-hex-*3*-yne-*2,5*-diol.

66-661;

## 1018: 2,4-DIMETHYLHEXEN-4-AL-6



$$CH_3-\underset{CH_3}{CH}-CH_2-\underset{CH_3}{C}=CH-CHO$$

$C_8H_{14}O = 126.20$

Colorless mobile liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful and, when undiluted, pungent, sweet-fatty-oily odor, in dilution more pleasant, almost fruity, herbaceous-Orange-like but with rather poor tenacity.

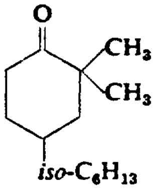
This aldehyde is rarely offered under its proper chemical name. It has been suggested for use in topnote compositions in perfumes of modern floral or aldehydic type. It blends well with Citrus notes and equally well with Rose and Jasmin notes, or Oriental-balsamic bases, e.g. Opopanax and Coriander.

It is, however, to the author's knowledge, very rarely used in creative perfumery. It finds a little use in the construction of artificial essential oils and flower absolutes.

Prod.: by condensation of Acetaldehyde with *2,4*-Dimethylbutanal.

3-190;

## 1019: 2,2-DIMETHYL-4-iso-HEXYLCYCLOHEXANONE



$C_{14}H_{26}O = 210.36$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Peculiar musky-woody odor with initial notes of rather harsh-chemical character.

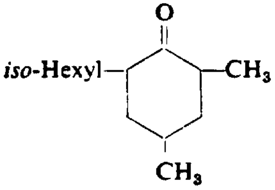
This chemical – together with the following four isomers – represent a further development of the ketones derived from Cyclohexanone in a long series of Dow Chem. Co. research chemical (mid-1950's).

Some of these new derivatives have achieved more popularity than others, and a few are sold under trade names.

They are particularly recommended for soap perfumes, detergents and other fragrances where power is imperative.

(See also: Parfumerie, Cosmetiques, Savons, Aug. 1965).

## 1020: 2,4-DIMETHYL-6-iso-HEXYL CYCLOHEXANONE



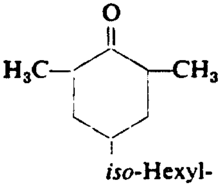
$C_{14}H_{26}O = 210.36$

Colorless liquid.

Powerful green-orrisy, slightly woody odor. Rather dry without being pronounced camphoraceous.

See notes under *2,2*-Dimethyl-*4*-*iso*-hexyl cyclohexanone.

## 1021: 2,6-DIMETHYL-4-iso-HEXYL CYCLOHEXANONE



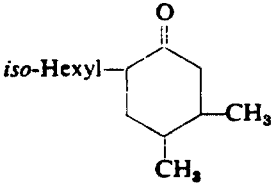
$C_{14}H_{26}O = 210.36$

Colorless liquid.

Musky-orrisy odor, somewhat sweeter than that of the *2,2*-Dimethylderivative, and less camphoraceous.

See notes under *2,2*-Dimethyl-*4*-*iso*-hexyl cyclohexanone.

## 1022: 3,4-DIMETHYL-6-iso-HEXYL CYCLOHEXANONE



$C_{14}H_{26}O = 210.36$

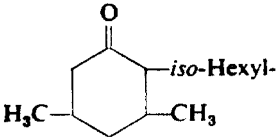
Colorless liquid.

Sweet-earthy, somewhat green-musty, also floral-orrisy odor with some resemblance to Vetiver.

This chemical is one of the more interesting of the series, and it may already be on many perfumers' shelves under a trade name.

See notes under *2,2*-Dimethyl-*4*-*iso*-hexyl cyclohexanone.

## **1023:** 3,5-**DIMETHYL**-2-iso-**HEXYL CYCLOHEXANONE**



$C_{14}H_{26}O = 210.36$

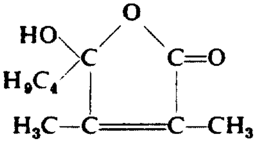
Colorless liquid.

Overall woody, orrisy with only a slight camphoraceous note, and with a peculiar fruity undertone that makes this derivative different from the other isomers.

See notes under *2,2*-Dimethyl-*4*-*iso*-hexyl cyclohexanone.

## **1024:** alpha-beta-**DIMETHYL**-gamma-**HYDROXY**-gamma-n-**BUTYL**-gamma-2-**BUTENOLIDE**

"Bovolide".
*2,3*-Dimethyl-*4*-keto-*2*-nonenoic acid, enol-lactone.



$C_{10}H_{16}O_3 = 184.24$

Colorless or very pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Very powerful, warm-herbaceous odor, often classified as Celery-like, but only pleasant in extreme dilution.

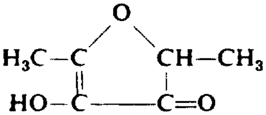
This Lactone, rarely available, occasionally manufactured by the immediate user, has found some use in flavor compositions, since it can help reproduce the odor of Butter and certain other dairy products.

It has been identified in butterfat at the concentration of 0.2 to 0.6 ppm. However, some authors still claim that the Lactones are formed from Hydroxyesters in the butterfat only after heat treatment.

159-674; 163-328;

## **1025:** 2,5-**DIMETHYL**-4-**HYDROXY**-3-(2H)-**FURANONE**

*4*-Hydroxy-*2,5*-dimethyl-*3*-(*2H*)-furanone.



$C_6H_8O_2 = 112.13$

Colorless or white crystals. M.P. 70° C.

Slightly soluble in water, soluble in alcohol and oils.

Intensely caramellic-fruity, "jam-like" odor with some resemblance to the odor of Palatone (Maltol). The odor is also reminiscent of that of "cooked Pineapple".

This chemical has been suggested for use in flavor compositions, primarily in imitation Pineapple, but also in Strawberry, Raspberry and various imitation "preserve"-type flavors.

It has been tentatively identified in Pineapple juice, but some doubt remains in the opinion of a few research workers who believe that this chemical may be formed during processing or during analysis of the juice.

It has been synthesized from *2,5*-Diacetyl-*3,4*-dihydroxy furan via several complicated steps. It is chemically related to the Lactone of Ribonic acid, commonly occurring in Nature.

In any event, it seems most conceivable that this material can become a very useful flavor material.

The concentration in finished products would probably be about 2 to 5 ppm.

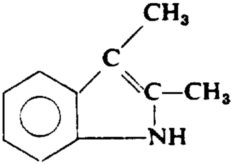
157-452; 157-458;
See also: 4th Food Symposium, Oregon State University, Sept. 1965 (Oregon, U.S.A.).
Journal of Org. Chemistry, vol. 31, July 1966, p. 2391-2395.

## 1026: DIMETHYL INDOLE

4 isomers are known and commercially produced:

*1,3*-Dimethyl indole.
*2,3*-Dimethylindole.
*2,5*-Dimethylindole.
*3,4*-Dimethylindole. (Was the first made).

The structure and description below refers to: *2,3*-Dimethylindole = *alpha-beta*-Dimethylindole ("Methylskatole").



$C_{10}H_{11} = 131.20$

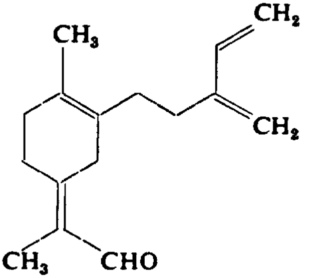
Colorless or white crystals. M.P. 56° C.

In extreme dilution of rather pleasant, sweet-floral odor, this Amine has only little of the "faecal" character commonly found in commercial grade Skatole (*beta*-Methylindole). The subject derivative is, however, considerably weaker and does not lend itself to any specific floral note, such as Indole (Jasmin-Gardenia, etc.). Difficulties in purifying the various isomers have also contributed to the reluctance in using or marketing these rare Indole derivatives.

69-84;

## 1027: 2,6-DIMETHYL-10-METHYLENE DODECA-2,6,11-TRIEN-1-AL

"Sinensal".



$C_{15}H_{22}O = 218.34$

Colorless liquid. B.P. higher than 300° C.

This aldehyde, only recently synthesized, has been suggested for use in perfume compositions, e. g. in the reconstruction of certain Citrus oils.

It is not yet commercially available, and it is still too early to make any statements as to the future of this material.

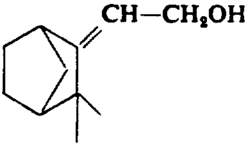
However, it is interesting to note that Methylene-citronellal (see that monograph) is an aldehyde with proven interest to the perfumer. It has a Methylene group located at an end position, although it is opposite of the Aldehyde group.

The title material is produced from Myrcene by oxidation. The alcohol thus formed is reacted with a Diene ether to yield above adduct after oxidation.

(See also: Soap, Perfumery & Cosmetics, June 1968, page 421-422).
158-128;

## 1028: 3,3-DIMETHYL-$\Delta^2$,beta-NORBORNANE-2-ETHANOL

"Camphene carbinol".



$C_{11}H_{18}O = 166.27$

Colorless, viscous liquid, solidifying in the cold.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

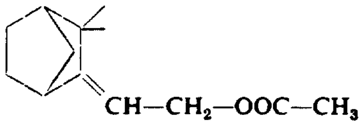
Sweet-camphoraceous, warm and soft odor with a woody undertone. Upon standing, it may develop an odor resembling that of Celluloid.

Although rarely offered commercially, this chemical could find some use in perfume compositions of the woody, Oriental and orrisy type, in new variations of Pine fragrances, and in various soap and detergent perfumes.

Prod.: from Cyclopentadiene.

## 1029: 3,3-**DIMETHYL**-Δ-2,beta-**NORBORNANE**-2-**ETHYLACETATE**

"Camphene carbinyl acetate".



$C_{13}H_{20}O_2 = 208.30$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Mild and sweet-woody odor with a floral-piney undertone. The commercial products are probably not very well-defined single chemicals, and great variations in odor have been observed.

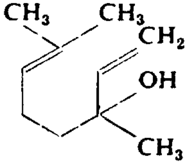
This ester has been developed in line with the research on Sandalwood type odors. The parent alcohol "Camphene carbinol" was once considered useful as a Sandalwood type material, but it has found more use as a sweetening and enriching ingredient in sophisticated Pine fragrances. The title ester finds limited use in perfume compositions of woody character, Fougeres, Pine fragrances, etc. and it blends very well with the Cyclohexanol derivatives, Ionones, *iso*-Bornylacetate, Nitromusks, etc.

Prod.: by acetylation of the carbinol.

## 1030: 3,7-**DIMETHYL**-1,6-**OCTADIEN**-3-**OL**

The above product is rarely offered as such but it occurs as one of two major components of Allo-ocimenol, commercially called "Muguol" (I.F. & F.)*)

These alcohols exists furthermore in *cis*- and *trans*-forms.



$C_{10}H_{18}O = 154.25$

Almost colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing and sweet, floral odor of moderate tenacity. The floral notes are accompanied by delicately citrusy notes resembling part of the lily odor complex.

The commercial product (mixture of two isomers) finds use in perfume compositions, mainly in soap and ordinary cosmetic fragrances, where its floral effect can be utilized more fully.

Several derivatives of "Muguol" are used in perfumery, some are even more commonly used than Muguol itself.

Prod.: from *alpha*-Pinene by pyrolysis to Allo-ocimene which is hydrated to the title material.

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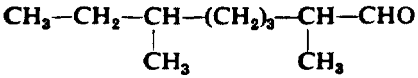
*) See also: Ocimenol (No. 2389).

## 1031: 2,6-DIMETHYL OCTANAL

*2,6*-Dimethyl octanoic aldehyde.
"*iso*-Decylaldehyde".
"*iso*-Aldehyde C-10".



$$CH_3-CH_2-\underset{CH_3}{\underset{|}{CH}}-(CH_2)_3-\underset{CH_3}{\underset{|}{CH}}-CHO$$

$C_{10}H_{20}O = 156.27$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Powerful, fresh, sweet and diffusive odor reminiscent of fruits and vegetables, overall greener and less fatty than Decanal.

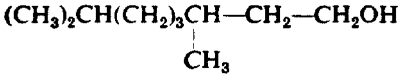
Rarely used in perfumery.

Finds some use in flavor compositions, e.g. for imitation Melon, etc., and the concentration would be mere traces.

G.R.A.S. F.E.M.A. No.2390.

## 1032: DIMETHYL OCTANOL

Tetrahydro geraniol.
Dihydro citronellol.
*3,7*-Dimethyloctanol-*1*.
Pelargol.
Rosidol.
D.M.O.
Rosorcol.
*2,6*-Dimethyloctan-*8*-ol.



$$(CH_3)_2CH(CH_2)_3\underset{CH_3}{\underset{|}{CH}}-CH_2-CH_2OH$$

$C_{10}H_{22}O = 158.28$

Colorless slightly oily liquid. B.P. 213° C. Sp.Gr. 0.83.

Almost insoluble in water and Glycerin. Soluble in alcohol, Propylene glycol and oils.

Waxy, dry-rosy odor. The description of this chemical has changed considerably over the past decade or so, because Dimethyl octanol was never commercially available in a state of purity that could justify any firm odor description. The typical waxy odor, the dry undertones, are more pronounced in purer grades. When made from synthetic Geraniol (Fritzsche Bros. and other manufact.) the D.M.O. is of high chemical purity and displays a more natural, waxy Rose-petal-like note.

Quite extensively used in perfume compositions, usually as a companion to Citronellol, Geraniol and Nerol, but in many cases the perfumer will deliberately avoid these other "Rose-alcohols" to emphasize the waxy or honeylike notes in a Rose base, and to make full use of the newer, purer Dimethyloctanol.

It finds use in flavor compositions, although only in the rarer types such as "floral", Rose, or various fruity flavors. The concentration in Ice cream will be about 50 ppm.

FCC-1964-817. G.R.A.S.
F.E.M.A. No.2391.

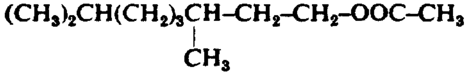
Prod.:

1) by reduction of Geraniol (synthetic or from Citronella oil).
2) by reduction of Citronellol, Citronellal or Citral.

4-43; 5-27; 86-44; 106-139; 155-130; 26-518; B-I-426; 103-234; 36-367;

## 1033: DIMETHYL OCTANYL ACETATE

Dihydrocitronellyl acetate.
Tetrahydrogeranyl acetate.
D.M.O. acetate.



$$(CH_3)_2CH(CH_2)_3\underset{CH_3}{\underset{|}{CH}}-CH_2-CH_2-OOC-CH_3$$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. B.P. 231° C.

Sweet floral-fruity, somewhat honey-waxy odor. Overall a pleasant and natural odor. Only its typical rosy notes prevent its wider application.

Finds use in perfume formulations as a modifier for Geranyl acetate, Citronellyl acetate and other esters, mainly in Rose compositions, and in soap perfumes of floral or sweet-fruity character.

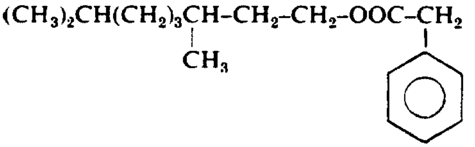
It remains, however, a comparatively rare chemical, and the author has the impression that the ester is simply non-existing in many perfume laboratories.

Prod.: by direct esterification of Dimethyl octanol with Acetic anhydride – or with Acetic acid under azeotropic conditions.

4-43; 86-44; 36-368;

## 1034: DIMETHYL OCTANYL PHENYLACETATE

D.M.O. phenylacetate.
Dihydrocitronellyl phenylacetate.
Tetrahydrogeranyl phenylacetate.



$C_{18}H_{28}O_2 = 276.42$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils. B.P. 340° C. Sp.Gr. 1.00.

Deep-sweet, rosy-tobacco-like odor with a faintly honey-like, floral undertone, the floral notes resembling the undertones in Jasmin.

Excellent base material for Rose bases of the "Rose absolute" type. Blends well with Trichloro methyl phenyl carbinyl acetate into highly fixative and extraordinarily tenacious compositions.

Although not offered from many manufacturers, this material has achieved some popularity among creative perfumers for its true-to-Nature Rose notes and for its versatility in blending pleasantly into fruity fragrances as well.

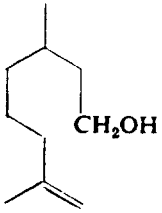
Occasionally used in flavor compositions of the fruity type, where its waxy-honey-like sweetness blends well into fruit-peel type flavors.

Prod.: from Dimethyl octanol and Phenylacetic acid in the presence of a catalyst, preferably under azeotropic conditions.

4-43; 36-368; 84-248; 77-194; 86-44; 86-48;

## 1035: DIMETHYL OCTENOL

"Rhodisol".
*3,7*-Dimethyl-*7*-octen-*1*-ol.
An isomer of Rhodinol (when that material is defined as -*6*-octen-*1*-ol).



$C_{10}H_{20}O = 156.27$

Colorless or very pale straw-colored oily liquid.

Almost insoluble in water, soluble in alcohol and oils, slightly soluble in Propylene glycol.

Sweet and rosy, oily odor of moderate to poor tenacity. Less "waxy" than the odor of Dimethyloctanol ("DMO"), but "fattier" and less tenacious, and with more initial power.

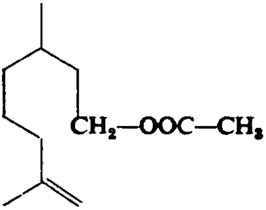
This alcohol, rarely offered under its proper chemical name, has been suggested for use in perfume formulations as a modifier for the conventional "rose alcohols". It lends more natural "oiliness" and it is quite powerful when compared to Citronellol and Dimethyloctanol. It tends to deteriorate under exposure to air, and this fact may contribute to the lack of interest on the part of the perfumers. Bottles of the material, unless frequently used, show resinification or polymerization around the stopper or neck, discouraging the perfumer from using such item.

The acetate – see next – is more stable and seems to have caught the interest of many perfumers.

See also: 4-125; 86-48;

## 1036: DIMETHYL OCTENYL ACETATE

*3*,*7*-Dimethyl-*7*-octen-*1*-yl acetate.



$C_{12}H_{22}O_2 = 198.31$

Colorless or very pale straw-colored liquid.

Slightly soluble in water, soluble in alcohol and oils, somewhat soluble in Propylene glycol.

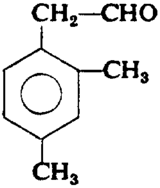
Sweet rosy-fruity odor with an oily-fruity undertone and moderate tenacity. The oily notes of the title material are not as typically Apple-like as those of Geranyl acetate.

This ester – rarely offered under its proper chemical name, except by one American producer – has found limited use in perfume compositions as a modifier for fruity-rosy fragrance types, particularly for detergent and soap fragrances, etc. It introduces rather pleasant freshness and attractive variations from the conventional rose theme.

It is furthermore interesting in Lavender compositions, many varieties of which have become quite successful in recent years' renaissance of Lavender modifications for men and women.

See also previous monograph: Dimethyl octenol.
(Fritzsche Bros. Inc. sample).

## 1037: 2,4-DIMETHYL PHENYLACETALDEHYDE



$C_{10}H_{12}O = 148.21$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful green, but sweet and slightly floral odor of moderate tenacity.

This aldehyde has been suggested for use in perfumery as a modifier for Phenylacetaldehyde in floral fragrances, where a green note is acceptable or desirable.

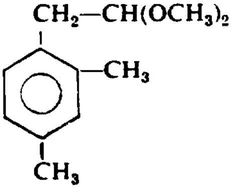
It does not have the penetrating power of Phenylacetaldehyde, but it is sweeter, more floral, less gassy and more tenacious. It is also somewhat more stable towards polymerization.

Prod.:

1) from *2*,*4*-Dimethyl phenylglycidic acid by decarboxylation.
2) from *2*,*4*-Dimethylbenzaldehyde plus Ethyl monochloroacetate via glycidate to the title material.

See also: Dimethyl phenylacetaldehyde diethylacetal (next monograph).

## **1038:** 2,4-**DIMETHYLPHENYLACETALDEHYDE DIETHYLACETAL**



$C_{12}H_{18}O_2 = 194.28$

Colorless or very pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild and delicately green-floral, sweet and tenacious odor.

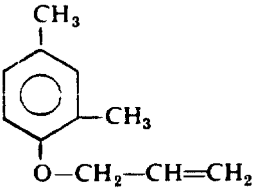
Very rarely offered commercially, this acetal has been suggested for use in Muguet, Lilac, Appleblossom and other floral fragrance types, where a discretely green note is desirable. It offers some advantage in being safe against attack from Methylanthranilate or Indole, two materials often used in such florals. The aldehyde itself (see previous monograph) would cause discoloration and odor change in presence of said Amines.

Prod. by condensation of the aldehyde with Ethanol, normally using dry Hydrogen chloride gas a condensing agent.

163-25;

## **1039:** ortho-para-**DIMETHYL PHENYLALLYLETHER**

*meta-4*-Xylenol allylether.



$C_{11}H_{14}O = 162.23$

Colorless mobile liquid. B.P. 220° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Sharp-herbaceous, remotely Geranium-like odor of moderate to poor tenacity. The odor is sweeter than that of Allyl phenyl ether (see monograph).

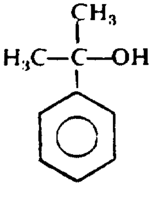
This material has occasionally been commercially available at very low cost, and subsequently found use in detergent and soap fragrances where power and low cost are imperative.

It does not offer – in the author's opinion – any unusual or very attractive notes other than what is obtainable with many common perfume materials. It seems most likely that this ether can be considered as obsolete within a decade or so.

Prod.: from *meta-4*-Xylenol plus Allyl bromide by heating in Acetone with dry Potassium carbonate in suspension.

## **1040: DIMETHYL PHENYL CARBINOL**

Phenyl-*iso*-propyl alcohol.
D.M.P.C.
Phenyl dimethyl carbinol.



$C_9H_{12}O = 136.20$

Crystalline, translucent mass, or white crystals, or slightly viscous, colorless liquid, solidifying in the cold.

Sp.Gr. 0.97 (liquid). M.P. 37° C.
B.P. 199° C. (slight decomposition).

Rosy-woody odor, somewhat fattier than that of Phenylethyl alcohol, and with a pleasant green-woody undertone. Overall drier and less floral than D.M.P.E.C. and much less green than Methyl phenyl carbinol.

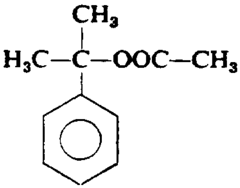
Interesting for woody tones in Rose bases, as a variation for Muguet and Lilac. It blends well with Ionones and Cedarwood derivatives for such purposes.

Prod.: by Grignard reaction on Acetone with Phenyl Magnesium bromide in Ether.

4-46; 5-68; 26-518; 34-162; 156-76; B-VI-506;

## 1041: DIMETHYL PHENYL CARBINYL ACETATE

D.M.P.C.A.
Phenyldimethyl carbinyl acetate.
Phenyl-*iso*-propyl acetate.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Fresh, green-spicy, slightly floral-fruity, yet sweet and very pleasant odor.

The taste resembles that of unripe plums (green skins of plums.).

Useful in perfumery for Clary Sage variations in Fougères, Chypres, Lavender compositions, and as a green-floral undertone and variant in Gardenia or Tuberose. It blends well with Dimethylbenzylcarbinol for Elderflower notes ("sureau") and builds good undertones in a Honeysuckle, etc.

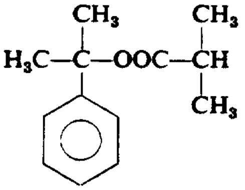
The unusual flavor of this chemical makes it valuable in Gooseberry, Rhubarb, Guava – all very difficult to imitate – and in Plum and Prune compositions.

Prod.: directly from Dimethyl phenylcarbinol and Acetic acid or Acetic anhydride.

4-46;

## 1042: DIMETHYL PHENYL CARBINYL-iso-BUTYRATE

*alpha-alpha*-Dimethylbenzyl-*iso*-butyrate.
Phenyldimethylcarbinyl-*iso*-butyrate.



$C_{13}H_{18}O_2 = 206.29$

Colorless, slightly oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-fruity, heavy, Apricot-Peach-Plum-like odor with a rather dry, woody-green undertone.

Somewhat green and slightly dry, Banana-Peach-Plum-like taste.

Finds some use in perfume compositions as a modifier for the carbinol or its acetate, e.g. in Chypre, Oriental or heavy floral or fruity composition. It blends very well with traces of Undecanolide, with Ionones and Linalool derivatives, etc.

Occasionally used in flavor compositions for imitation Banana, Apricot, Peach, etc.

The concentration in Icecream would be about 40 ppm or less.

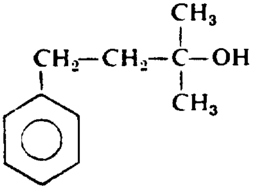
Prod.: by direct esterification of Dimethylphenylcarbinol with *iso*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2388.

NOTE: The author believes that subject chemical is occasionally confused with Dimethyl phenyl*ethyl* carbinyl *iso*-butyrate which is, in the author's opinion, a superior material as far as odor and flavor beauty is concerned. Literature seems to indicate that descriptions of D.M.P.C. and its esters in many cases are actually descriptions of D.M.P.E.C. and its esters.

## 1043: DIMETHYL PHENYLETHYL CARBINOL

"Centifol".
D.M.P.E.C.
*beta*-Phenylethyl dimethyl carbinol.
*1,1*-Dimethyl-*3*-phenylpropanol-*1*.



$C_{11}H_{16}O = 164.25$

Colorless viscous liquid. B.P. 238° C. Sp.Gr. 0.97.

A certain modification of this chemical is solid at room temperature and melts at 30° C.

Very slightly soluble in water, soluble in alcohol and oils.

Soft, floral-green, mildly herbaceous and oily odor reminiscent of Lily and Hyacinth, but with an unusual mildness in spite of great tenacity. Probably the most valuable and versatile of all the so-called "carbinols".

An excellent blender and background in many florals, from Rose and Jasmin to Muguet and Magnolia, at the same time powerful and delicate. It introduces an excellent undertone and base in Chypres and other non-florals.

Combining the best of Linalool and Terpineol – without the volatility of Linalool and without the woody-piney notes of Terpineol – it has but one disadvantage: a rather high price. Too high for volume use in everyday perfumery. But increased demand and use has already brought the cost within reasonable limits.

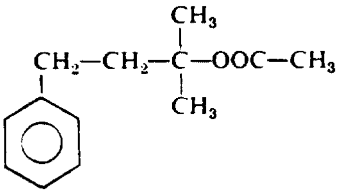
Concentrations from 1 or 2% up to 30% are known and show the versatility and overall agreeable odor type of this chemical.

Prod.: from Phenylethyl Magnesium bromide (or Chloride) with Acetone by Grignard reaction.

4-115; 5-67; 31-23; 34-162; 4-46; 86-48; 156-77; 103-291;

## 1044: DIMETHYL PHENYLETHYL CARBINYL ACETATE

D.M.P.E.C. acetate.
Phenylethyl dimethylcarbinyl acetate.
*2*-Methyl-*4*-phenyl-*2*-butylacetate.
Centifolin.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 244 C. Sp.Gr. 0.99.

Fresh and rosy, slightly leafy-fruity and tenacious odor. Overall floral in the Rose-Hyacinth-Jasmin type with a balsamic undertone of pleasant softness.

A very useful material in perfumery. It introduces fullness ("body") and intensifies the delicate floral notes of Rose, Jasmin, Lily, etc. without making them appear harsh or offensive. It gives impression of deepness in odor, richness in fragrance.

Finds some use in flavor compositions, mainly in Tea-like fruity compositions, Strawberry, etc. In flavors, too, it lends great depth and richness even at very low concentrations. The material would appear at about 0.5 to 10 ppm in the finished product.

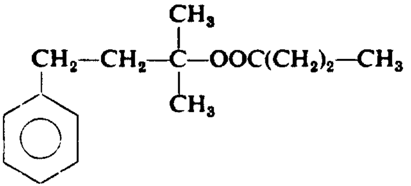
Prod. by direct esterification of Dimethylphenylethyl carbinol with Acetic acid or Acetic anhydride.

G.R.A.S. F.E.M.A. No.2735.

4-115; 4-46; 5-67; 33-504; 34-162; 156-76; 103-292;

## 1045: DIMETHYL PHENYLETHYL CARBINYL-n-BUTYRATE

D.M.P.E.C. butyrate.
Phenylethyl dimethylcarbinyl-*n*-butyrate.



$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 253° C.

Sweet-herbaceous, Tea-like and Clary-Sage-like odor of great tenacity and very pleasant overall character. The undertones are slightly fruity and tobacco-like, giving a very "natural" impression. It represents one of rather few aromatic chemicals that have a "natural" odor and even in perfumery/olfactory grade of purity show a complex equal to a pleasant perfume composition.

Needless to add, that for an odor description as the one given above, the material must be free from Butyric acid traces. Once it is produced in an acid-free grade, it keeps remarkably well under normal laboratory storage conditions.

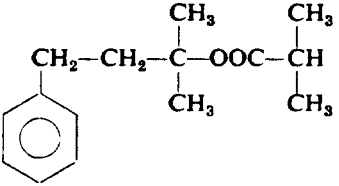
Finds use in Rose, Sweet-Pea, Chypre and Fantasy type perfumes. Gives interesting effects in flavor compositions, mainly as an amplifier in Berry flavors and Prune/Plum type flavors. The industry has, however, concentrated upon the use of the *iso*-Butyric ester (see next) and the above described ester is not even listed as G.R.A.S. in the Federal Register (U.S.A.).

Prod.: by direct esterification of Dimethylphenylethylcarbinol with *n*-Butyric acid under azeotropic conditions. Careful drying and neutralization of the vacuumdistilled ester.

86-48;

## 1046: DIMETHYL PHENYLETHYL CARBINYL-iso-BUTYRATE

D.M.P.E.C.-*iso*-butyrate.
Phenylethyl dimethylcarbinyl-*iso*-butyrate.
*2*-Methyl-*4*-phenyl-*2*-butyl-*iso*-butyrate.



$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 250° C.

Peculiar fruity-juicy, Tea-like and herbaceous, richly sweet odor, overall refreshing and somewhat reminiscent of the odor of Carob beans – without the cheesy notes of that material.

Interesting in perfumery for Chypre, Fougère, Lavender, Rose, Fantasy, etc. It is less complex and also less "natural" than the *n*-Butyrate, but in a way it presents a "cleaner" odor, not quite as heavy as that of the *n*-Butyrate.

Finds some use in flavor compositions for imitation fruit, Melon, Berry-types, Cherry, Plum, etc.

The concentration in finished products will normally be about 0.5 to 50 ppm. Like the parent carbinol, this ester has wide limits of concentration-application, showing the overall acceptability of this odor/flavor type.

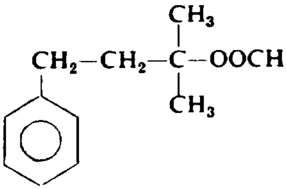
Prod.: by direct esterification of Dimethylphenylethylcarbinol with *iso*-Butyric acid or *iso*-Butyric anhydride. In the former case, preferably under azeotropic conditions. This ester is considerably more stable than the *n*-Butyric ester with respect to hydrolysis (or "acid" notes).

G.R.A.S. F.E.M.A. No.2736.

4-46; 4-115; 34-162; 86-48; 156-76;

## 1047: DIMETHYL PHENYLETHYL CARBINYL FORMATE

D.M.P.E.C. formate.
Phenylethyl dimethylcarbinyl formate.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. B.P. 241° C.

Almost insoluble in water, soluble in alcohol and oils.

Dry, floral-rosy odor with emphasis upon Rose-foliage notes.

Interesting perfume material for Hyacinth, Chypre, Fougère and for variations in Rose.

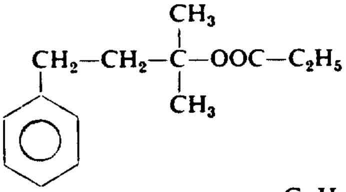
Has been suggested for Berry and vegetable type of flavors.

Perhaps because of the poorer grade of occasional commercial lots of this chemical, it has never achieved much popularity. However, it is quite possible to manufacture this material in an acid-free and reasonably stable grade. Such material displays very interesting odor characteristics, worthwhile making use of.

Prod.: from Dimethylphenylethylcarbinol and Formic acid with the aid of Acetic anhydride.

## 1048: DIMETHYL PHENYLETHYL CARBINYL PROPIONATE

D.M.P.E.C. propionate.
Phenylethyl dimethylcarbinyl propionate.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 249° C.

Sweet, fruity-herbaceous Mirabelle-like odor (sweet, non-almondy Cherry type of odor).

Pleasant, rich-fruity taste, reminiscent of berries, Plums, etc.

Useful in perfume compositions for Rose, Sweet-Pea, Freesia, Peony, Magnolia and many other types of delicate and sweet or fruity florals. It has excellent tenacity and stability, and blends well with the conventional fragrance materials for these types.

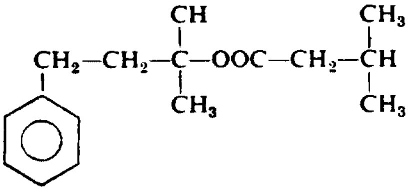
In flavor compositions, it finds use for Mirabelle (a fresh, juicy-berry-like Plum-Cherry fruit), in Plum or Prune compositions and in many types of berry flavors.

Prod.: by direct esterification of Dimethylphenylethylcarbinol with Propionic acid (azeotropic conditions) or with Propionic anhydride.

86-48;

## 1049: DIMETHYL PHENYLETHYL CARBINYL-iso-VALERATE

D.M.P.E.C.-*iso*-valerate.
Phenylethyl dimethylcarbinyl-*iso*-valerate.



$C_{16}H_{24}O_2 = 248.37$

Colorless liquid. Insoluble in water, soluble in alcohol and oils. B.P. 259° C.

Green-floral, very "juicy" odor of remarkable "naturalness" and complexity.

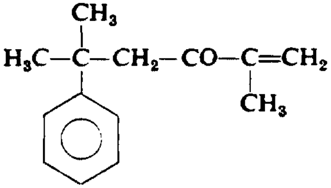
Interesting item for Fougères, floral fragrances, Chypres, etc. particularly with Clary Sage, which it resembles much in odor effect.

When absolutely free from *iso*-Valeric acid, it has extremely pleasant character and richness in odor picture.

Occasionally used in flavor compositions, e.g. for Apple flavors.

Prod.: by direct esterification of Dimethylphenylethylcarbinol with *iso*-Valeric acid under azeotropic conditions. Thorough neutralization, and drying of the vacuumdistilled ester.

## 1050: 2,5-DIMETHYL-5-PHENYL-1-HEXEN-3-ONE



$C_{14}H_{18}O = 202.30$

Colorless, slightly viscous liquid. Almost insoluble in water, soluble in alcohol and oils.

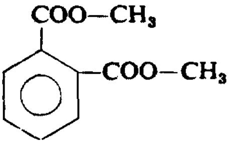
Dry-woody-rosy odor of fair tenacity. Powerful, but displays some camphoraceousness in its overtones, partly ruining the fragrance picture.

Rarely offered commercially under its chemical name, this material has been suggested for use in Rose bases and in general as a modifier for the conventional Rose materials.

Prod.: by condensation of Phenyl dimethylcarbinol with Methyl-*iso*-propenylketone (from Methyl ethyl ketone plus Paraformaldehyde).

## 1051: DIMETHYL PHTHALATE

Dimethyl-*ortho*-phthalate.
Methyl phthalate.
D.M.P.
Avolin (Fritzsche Bros.).
Palatinol M.
Mipax.
Fermine.
Solvarom.



$C_{10}H_{10}O_4 = 194.19$

Colorless oily liquid. Sp.Gr. 1.19.
B.P. 284° C.

0.4% soluble in water, almost insoluble in hydrocarbons (Terpenes, Mineral oil, etc.), soluble in alcohol and perfume oils. Solidifies in the cold, the pure material melts at 6° C. Very faint, ethereal odor. It has been claimed that the material is virtually odorless, but that it hydrolyzes easily, producing a faint odor of Methanol.

Has been used as a solvent in perfumery, but is now practically abandoned for that purpose (substituted by Diethyl phthalate).

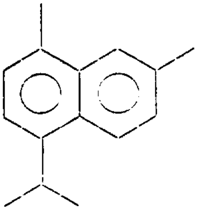
Was introduced in the 1940's as an insect repellant with specific effect against mosquitoes. However, it is comparatively toxic and acts as a Central Nervous System depressant upon the human being. The hydrolysis of the ester in actual use upon the human skin is therefore a distinct disadvantage.

Prod.: from Phthalic anhydride and Methanol.

4-46; 26-518; 86-48; 95-187; 100-372;
B-IX-797;

## 1052: 1,7-DIMETHYL-4-iso-PROPYL NAPHTHALENE

*iso*-Cadalin.



$C_{15}H_{18} = 198.31$

Colorless, slightly viscous liquid.
B.P. 262° C.

Practically insoluble in water, soluble in alcohol and oils.

Dry-musty, woody and very tenacious odor of some similarity to the dry notes in Ambregris.

The title material is briefly mentioned as an example of a series of chemicals developed in the early 1920's by a perfumery research team including Professor Ruzicka, later Nobel laureate.

The material has long since experienced its culmination of success as an Ambregris chemical, while newer and more true-to-Nature materials have been developed in the past decade.

However, the title material is interesting in its origin and it represents a milestone in organic chemistry, particularly for the chemistry of the sesquiterpenoids.

Prod.: by dehydrogenation of Carotol, a sesquiterpenoid alcohol obtained from Carrot seed oil. The world market was thoroughly upset at one time in 1959, when an unidentified customer made an inquiry for 600 kilos of Carrot seed oil, and the perfume industry was wondering: for which purpose?

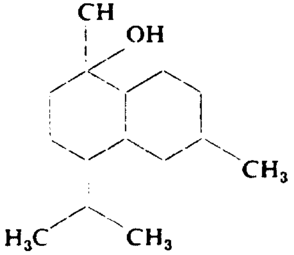
The sesquiterpene Cadinene will yield Cadalene (the *1,6*-isomer of the title material) by dehydrogenation.

Eudesmol yields *1*-Methyl-*7*-*iso*-propylnaphthalene, also called Eudalene. Vetivone yields Vetivalene = *1,5*-Dimethyl-*3*-*iso*-propylnaphthalene.

1-719; 67-632; 67-671; 68-1288; 87-250; 88-297; 87-265;
See also: *1,6*-Dimethyl-*4*-*iso*-propyl-oxy-decahydronaphthalene.

## 1053: 1,6-DIMETHYL-4-iso-PROPYL-OXY-DECAHYDRONAPHTHALENE

The title name is misleading, but commercially used for the chemical:
*1,6*-Dimethyl-*4*-*iso*-propyldecalinol.
Dihydro cadinol.



$C_{15}H_{28}O = 224.39$

Colorless or white crystals. M.P. 130° C.

Insoluble in water, soluble in alcohol and oils.

Powerful and very dry, musty-woody odor of similarity to the dry notes of Ambregris. In proper dilution, the dry notes become more pleasant, and they do not display any phenolic, medicinal or tarry character. The tenacity is excellent, and the power of this material is often underestimated.

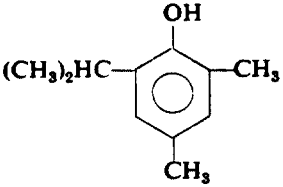
The title material is rarely offered commercially, but it has been used with success in various specialties, not always Ambregris bases. Its power can be used to give "lift" to a number of non-floral fragrance types, and in combination with Galbanum, Oakmoss, etc. it may form a very important part of certain types of luxury perfume.

Prod.: by catalytic hydrogenation of Cadinols.

67-664; 88-260;
See also monograph: *1,7*-Dimethyl-*4*-*iso*-propyl naphthalene.

## 1054: 2,4-DIMETHYL-6-iso-PROPYLPHENOL

*5-iso*-Propyl-*meta-4*-xylenol.
*2-iso*-Propyl-*4,5*-dimethylphenol.



$C_{11}H_{16}O = 164.25$

White crystalline powder or granular crystals.

Insoluble in water, poorly soluble in aqueous alkali, soluble in alcohol and miscible with most oils.

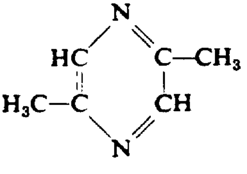
Powerful, tenacious and warm, spicy-herbaceous odor, often compared to that of Safran (Saffron). The author finds more resemblance to Oakmoss.

This rare chemical has been suggested for use in perfume compositions where warm-herbaceous and mildly spicy odors are desirable, or modifications of such odors wanted. It does not, in the author's opinion, substitute Safran in an established formula, but it does introduce interesting notes in Ambre compositions and bases, etc. As a modifier in Fougère and Chypre compositions, it makes pleasant changes in the conventional Oakmoss notes.

4-45; (see also 68-423;) 163-211;

## 1055: 2,5-DIMETHYL PYRAZINE

Glycoline.
Ketine.
*2,5*-Dimethyl-*1,4*-diazine.



$C_6H_8N_2 = 108.15$

Colorless liquid, solidifying in the cold, melting at 15° C. Sp.Gr. 0.99. B.P. 153° C.

Miscible with water (in neutral solution), miscible with alcohol and most flavor oils.

Reacts with aldehydes and some ketones.

Has been identified in the volatile components of roasted coffee.

This material is held chiefly responsible for the typical flavor of Potato Chips (oil-fried, thin-sliced Potato). It has therefore been manufactured synthetically and is used in the reconditioning of commercial products, such as Potato Chips and the packaging material for same, and also for reconditioning of "instant" coffee.

To the author's knowledge, it has no other mission in flavors or perfumes.

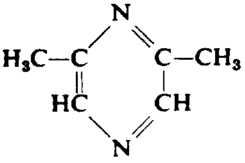
Prod.:

1) from Amino-acetone by self-condensation, followed by oxidation with Mercury chloride.
2) by heating Glycerin with Ammonia salts, producing Acrolein and Ammonia.
3) from Ethyl-*alpha*-aminoacetate, treated with Copper sulfate.

26-518; 69-1321; B-XXIII-96; 157-377; 157-443;

## 1056: 2,6-DIMETHYL PYRAZINE

*2,6*-Dimethyl-*1,4*-diazine.



$C_6H_8N_2 = 108.15$

White crystals. M.P. 48° C. B.P. 155° C.

Soluble in water (neutral solution), soluble in alcohol and most flavor oils. Reacts with aldehydes and some ketones.

Sweet, "fried" odor, resembling that of fried Potatoes, but not as typical as that of the *2,5*-isomer (see previous monograph).

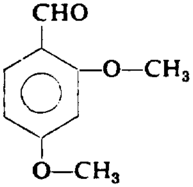
Has been suggested for use in flavors for reconditioning of the aroma of potato chips, "instant" coffee, etc.

Prod.: From Glucose and Ammonia.

69-1321; 157-443;

## 1057: para-DIMETHYL RESORCYLIC ALDEHYDE

*beta*-Resorcylaldehyde dimethylether.
*2,4*-Dimethoxybenzaldehyde.
*2*-Methoxy anisaldehyde.



$C_9H_{10}O_3 = 166.18$

White or colorless needlelike crystals.
M.P. 70° C. B.P. 265° C.

Insoluble in water, soluble in alcohol and oils.

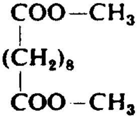
Although this aldehyde is so closely related to common and popular perfume chemicals, it has failed to achieve interest among the perfumers. Apparently a result from research on Oakmoss chemicals, this Alkoxyaldehyde has only a faint, sweet Nut-like and remotely floral odor of considerable tenacity; remotely reminiscent of Heliotrope. Most conceivably, its high boiling point (and low vapor pressure) contribute to the apparent lack of power in its odor. It lends some fixative effect, and it has occasionally been used in perfume compositions as a modifier for Anisaldehyde, etc. in Chypres, Fougeres and similar heavy complexes. Otherwise, the material is generally unknown to most perfume laboratories.

Prod.: by Tiemann-Reimer reaction (formation of phenolic aldehydes from Phenol + Chloroform + Alkali) upon Resorcinol, followed by Methylation with Dimethylsulfate. Also from Resorcinol with Hydrocyanic acid or with Hydrochloric acid, followed by Methylation.

26-512; 160-826; B-VIII-242; see also: 68-748; 61-60;

## 1058: DIMETHYL SEBACATE

Dimethyl decane dioate.
Methyl sebacate.
*1,8*-Octanedicarboxylic acid, dimethylester.



$$\begin{array}{l} COO-CH_3 \\ | \\ (CH_2)_8 \\ | \\ COO-CH_3 \end{array}$$

$C_{12}H_{22}O_4 = 230.31$

Needle-like or plate-like colorless or white crystals. M.P. 38° C. B.P. 293° C.
Sp.Gr. 0.99 (liquid).

The liquid material is colorless.

Pleasant and mild-ethereal-fruity odor.

Fruity-winey, ethereal Apple-like taste, but very mild.

Has been used as a solvent in perfume compositions, but is now rarely used for that purpose.

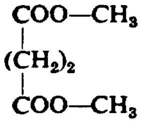
Finds some use in flavor compositions, mainly in imitation Apple, Brandy, Wine, Melon, etc.

Prod.: by direct esterification of Sebacic acid and Methanol, usually under azeotropic conditions.

4-96; 26-520; 77-189; B-II-293, zweiter Ergzbd.;

## 1059: DIMETHYL SUCCINATE

Methyl succinate.
Methyl butanedioate.



$$\begin{array}{l} COO{-}CH_3 \\ | \\ (CH_2)_2 \\ | \\ COO{-}CH_3 \end{array}$$

$C_6H_{10}O_4 = 146.15$

Colorless liquid, solidifying in the cold.
M.P. 19° C. Sp.Gr. 1.12. B.P. 195° C.

1 % soluble in water, 3 % soluble in alcohol, miscible with oils.

Pleasant ethereal-winey, dry-green, slightly fruity odor. Winey, but somewhat burning taste.

Finds some use in flavor compositions, particularly in imitation Rum, Strawberry, Blackcurrant, Gooseberry, etc.

The concentration in the finished product may be as high as 100 ppm (in soft drinks and other beverages).

G.R.A.S. F.E.M.A. No.2396.

Prod.: directly from Methanol by esterification with Succinic acid under azeotropic conditions.

26-520; 66-970; 100-683; B-II-609;
see also: 77-189;

## 1060: DIMETHYL SULFIDE

Methyl sulfide.

$(CH_3)_2S$

$C_2H_6S = 62.14$

Almost colorless oily liquid. B.P. 37° C.
Sp.Gr. 0.85.

Insoluble in water, soluble in alcohol and oils.

Extremely diffusive, repulsive odor, reminiscent of wild Radish, sharp, green, Cabbage-like. Only in very high dilution it becomes bearable and almost acceptable, pleasant, vegetable-like.

Finds a little use in perfumery, mainly in the reconstruction of certain essential oils (Geranium, Peppermint, etc.).

Occasionally used in flavor compositions, for imitation Coffee, Chocolate, Cocoa, Molasses (caramel-treacle) and certain fruit types.

The concentration will usually be as low as 0.1 to 2 ppm in the finished consumer product.

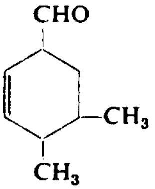
G.R.A.S. F.E.M.A. No.2746.

Prod.: from Potassium methylsulfate plus Potassium sulfide.

26-520; 65-730; 90-824; 100-683; 158-181;
B-I-288; 140-176;

## 1061: 3,4-DIMETHYL-Δ5-TETRAHYDROBENZALDEHYDE

*3,4*-Dimethyl cyclohex-*5*-enyl carboxaldehyde.



$C_9H_{14}O = 138.21$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, green and rather dry-waxy, but in dilution very refreshing odor of moderate tenacity. It lacks natural character, but is rarely used as the "only aldehydic" component of any refreshing topnote or Aldehyde note.

The title aldehyde, related to Safranal (*2,6,6*-Trimethyl-) has found some use in perfume compositions as a powerful and refreshing ingredient with Citrus notes or woody notes. It is fairly stable in ordinary soap, and blends well with Cedarwood derivatives, Ionones, etc.

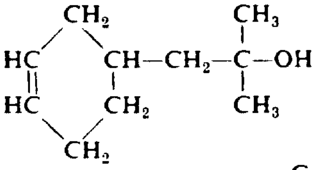
Interesting ketones have been prepared by condensing the subject aldehyde with Acetone in reactions similar to those used in the preparation of Ionones. The resulting alkyl-substituted Tetrahydrobenzylidene butenones or their corresponding, hydrogenated products often possess great sweetness and interesting character.

This aldehyde is rarely offered under its proper chemical name.

See also: Dimethyl butadieneacrolein.

## 1062: DIMETHYL TETRAHYDROPHENYLETHYL ALCOHOL

"Moscatol".
*alpha-alpha*-Dimethyl-*beta*-cyclohexen-*3*-yl ethanol.
A tertiary alcohol, chemically related to the Silveterpineols.
Tetrahydro dimethylbenzyl carbinol.



$C_{10}H_{18}O = 154.25$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-camphoraceous, heavy-anisic or Sassafras-like herbaceous odor with pronounced musky-animal undertones and considerable tenacity.

This rare chemical, identified in the essential oil from the leaves of a Chilean tree, has found some use in perfumes, particularly for soap. Several "specialties" are based wholly or partially upon this chemical and sold under various trade names, usually employing the name "musk" in one form or another.

The odor type is rather unusual for a tertiary alcohol. Such alcohols, particularly when connected to a Cyclohexane Cyclohexene ring system, will normally have very dry, camphoraceous, woody and or green odors.

Prod.: by isolation from the essential oil of leaves from a tree, indigenous to Chile.

86-99;

## 1063: DIMETHYL TETRASULFIDE

$CH_3—S—S—S—S—CH_3$

$C_2H_6S_4 = 158.33$

Pale yellowish mobile oil.

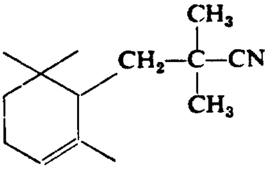
Powerful and penetrating Onion-like odor, in extreme dilution almost pleasantly green, vegetable-leafy and sweet.

This sulfide, rarely offered commercially, has found very limited use in the reconstruction of certain essential oils, and in minute traces as a component of novel topnote compositions.

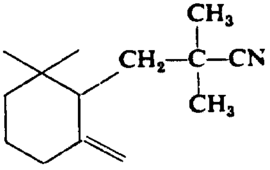
It is also used to a limited degree in flavor compositions, ranging from Coffee imitation to Onion or imitation "vegetable" flavors.

## 1064: 2,2-DIMETHYL-3-(2,6,6-TRIMETHYL-2-CYCLOHEXEN-1-YL)-PROPIONITRILE

The commercial product will normally contain a considerable amount of *gamma*-isomer. The title name represents the *alpha*-isomer.



*alpha*-isomer



*gamma*-isomer

$C_{14}H_{23}N = 205.35$

Colorless or very pale straw-colored liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and floral, rather pungent odor, in dilution with balsamic undertones, more woody-floral, moderately tenacious.

This Nitrile, developed in search of useful counterparts to the earlier developed Geranyl butyraldehyde, has been suggested for use in perfume compositions as a floral-woody modifier.

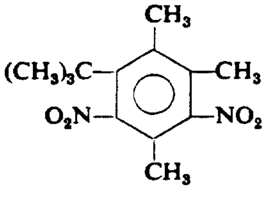
Its greater stability in mildly alkaline media gives it certain advantages over the aldehyde-type materials, while this Nitrile (and other Nitriles) is not absolutely free from hazard of decomposing.

It is therefore most likely that the title material will remain relatively unknown, and not become a standard item. Its olfactory virtues are not conspicuous enough to justify general recommendation of the item.

Prod.: from Geranyl-*iso*-butyronitrile by cyclization, normally with Phosphoric acid.

## 1065: DINITRO-tertiary-BUTYL PSEUDO CUMENE

*1*,*2*,*4*-Trimethyl-*3*,*5*-dinitro-*6*-*tertiary*-butylbenzene.



$C_{13}H_{18}N_2O_4 = 266.30$

Yellowish crystals. M.P. 137° C.

Insoluble in water, poorly soluble in alcohol, soluble in most perfume oils.

Sweet and tenacious odor resembling that of Musk Ketone, but somewhat sharper yet not quite as powerful.

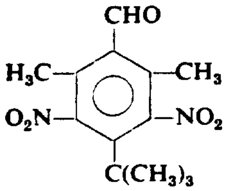
Has been suggested for use in perfume compositions, but this material does not have any distinct advantages over the conventional Nitromusks, and it can be considered more or less obsolete now.

Prod.: from *tertiary*-Butylalcohol and Pseudocumene followed by Nitration.

5-302;

## 1066: DINITRO-tertiary-BUTYL XYLENE ALDEHYDE

Dinitro dimethyl butyl benzaldehyde.
"Musk Aldehyde".
"Aldehydmoskus".



$C_{13}H_{16}N_2O_4$ = 264.19

Pale yellowish crystals. M.P. 112° C.

Insoluble in water, poorly soluble in alcohol, soluble in most perfume oils.

Sweet musky odor, reminiscent of Musk Xylol, but not quite as harsh, and not quite as strong.

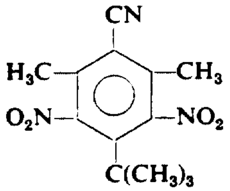
This Nitromusk – one of the original "Baur Musks" can be classified as practically obsolete, brought out of use by superior Nitromusks and later by even more superior Indane-, Chromane or Tetralin musks, Macrocyclic musks, etc.

Prod.: from *2,4*-Dimethyl-*6-tertiary*-butylphenyl glyoxylic acid plus Toluidine followed by Nitration of the aldehyde.

5-299; 5-302; 95-197; 96-230;

## 1067: DINITRO-tertiary-BUTYL XYLYL CYANIDE

"Musk Cyanide".
*3,5*-Dinitro-*2,6*-dimethyl-*4-tertiary*-butylbenzonitrile.



$C_{13}H_{15}N_3O_4$ = 277.29

Prismatic, pale yellowish crystals.
M.P. 110° C.

Insoluble in water, slightly soluble in alcohol, soluble in most perfume oils.

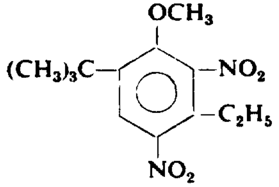
The odor of this Nitromusk resembles that of the previous musk (Musk Aldehyde).

Practically abandoned in modern perfumery.

5-299; 5-302; 95-197; 96-230;

## 1068: 2,4-DINITRO-3-ETHYL-6-tertiary-BUTYLANISOLE

"Homo-Ambrettemusk".
"Homo Musk Ambrette".



$C_{13}H_{18}N_2O_5$ = 282.30

Yellowish granular crystals.

Insoluble in water, poorly soluble in alcohol, moderately soluble in oils and common perfume solvents.

Sweet and tenacious musky odor. The type is inbetween Musk Ambrette and Musk Ketone, but weaker than both.

This Nitromusk was developed among scores of derivatives in search of more interesting Musk odorants in the same price-class as the conventional Nitromusks. Only a few

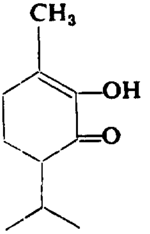
Nitromusks have had succes in remaining on the perfumer's shelf in competition with the nearly century-old Nitromusks, and the title material is not one of the more successful ones.

It has had some use and its advantage was in the lesser tendency of discoloring under exposure to daylight, a drawback strongly in disfavor of the conventional Nitromusks.

Prod.: from *tertiary*-Butyl-*3*-methoxyethylbenzene by Nitration.

## 1069: DIOSPHENOL

*2*-Hydroxypiperitone.
Buchu camphor.
*1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*2*-ol-*3*-one.
*1*-*para*-Menthen-*2*-ol-*3*-one.



$C_{10}H_{16}O_2 = 168.24$

Colorless or white crystals. M.P. 83° C. Sp.Gr. 0.95 (liquid. B.P. 233° C. (decomposition).

Powerful minty, somewhat Tea-like, herbaceous odor.

This material tends to oxidize so easily that it is a hindrance to its wider use in perfumery.

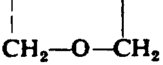
Has occasionally found use in flavor compositions, years ago in various toothpaste flavor compositions, but the author believes that the use of Diosphenol in flavors has been practically abandoned. The natural oil, Buchu leaf oil, is still used in various types of Mint flavor, particularly in Europe and South Africa.

Prod.: by isolation from Buchu leaf oil (crystallization).

67-529; 90-7; 100-378; 104-107;

## 1070: DIOXANE

Dioxan.
*1*,*4*-Diethylene dioxide.
Dioxane-*1*,*4*.



$$\begin{array}{l} CH_2{-}O{-}CH_2 \\ |\qquad\quad\;\; | \\ CH_2{-}O{-}CH_2 \end{array}$$

$C_4H_8O_2 = 88.11$

Colorless liquid, solidifying in the cold.
M.P. 12° C. Sp.Gr. 1.04. B.P. 101° C.

Hygroscopic and miscible with water. Soluble in alcohol and oils.

Very sweet, mild-ethereal odor.

Although not directly a perfume material, this chemical is mentioned because it occasionally is used as an extraction solvent for perfume raw materials. Traces of the solvent may remain in the commercial product and influence the odor of the natural extract.

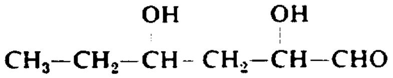
Certain derivatives of Dioxan (cyclic glycol acetals) are used in perfumes and flavors. Dioxane is slightly toxic in its effect upon the human Central Nervous System. It is also flammable and presents a fire hazard.

Prod.: by Etherification (dehydration) of Ethylene glycol.

26-502; 31-149; 69-1528; B-IV-255; 1-249; 100-378;

## 1071: alpha-gamma-**DIOXY**-n-**CAPROIC ALDEHYDE**

*2,4*-Dihydroxyhexanal.



$CH_3-CH_2-\overset{OH}{CH}-CH_2-\overset{OH}{CH}-CHO$

$C_6H_{12}O_3 = 132.16$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and refreshing, green-lemony, herbal odor of moderate to poor tenacity.

This aldehyde is rarely, if ever, marketed under its chemical name, but it has found some use in perfume compositions, mainly as part of the topnote in Citrus colognes, light or green floral fragrances, etc.

It blends very well with all Citrus oils, with the "rose alcohols" and Hydroxycitronellal, Neroli and Petitgrain, etc. and it offers interesting notes for composition of "aldehydic topnote bases" which are still very fashionable.

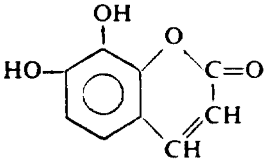
Prod.: from Sorbic aldehyde.

See also monograph: *gamma*-Hydroxy caproic aldehyde.

## 1072: 7,8-**DIOXYCOUMARIN**

Daphnetin.

Trihydroxycinnamic acid, *delta*-lactone.



$C_9H_6O_4 = 178.15$

Yellowish crystals. M.P. 256° C.

Almost insoluble in cold water. Slightly soluble in boiling water. Poorly soluble in alcohol and oils.

Faint and sweet-herbaceous, slightly woody-tobacco-like odor, reminiscent of the odor of Coumarin, but much weaker.

This chemical has, to the author's knowledge, no application in perfumes or flavors, but it is occasionally used as a sunscreening agent. Since it has an odor, it is briefly described here. It may at times influence the odor of a perfume used in a cosmetic preparation containing Dioxycoumarin.

Prod.: by enzymatic hydrolysis of Daphnin (a glucoside from the bark of Daphne mezereum).

or: by synthesis from Pyrogallaldehyde (Perkin's reaction).

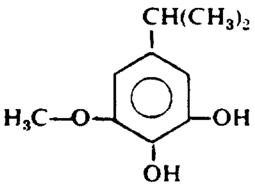
100-319; 68-1011;

## 1073: 3,4-**DIOXY**-5-**METHOXY**-iso-**PROPYLBENZENE**

Methoxy-*iso*-divarinol.

*3,4*-Dihydroxy-*5*-methoxy-*1*-*iso*-propylbenzene.

*5*-*iso*-Propyl-*3*-methoxy pyrogallol.



$C_{10}H_{14}O_3 = 182.22$

White crystals, darkening under exposure to air.

Very dry, tarry-smokey odor of considerable tenacity. Upon dilution it develops a sweeter and much more pleasant mossy-dry odor of considerable resemblance to notes in certain types of Oakmoss extract.

Closely related to chemicals occurring in Nature and to components of Birch tar oil, this Phenolether has been suggested for use in perfume compositions of the non-floral type.

It lends considerable power and "lift" to mossy or dry-woody notes and blends excellently with Eugenolderivatives, Oakmoss, Ionones, Amylsalicylate, Labdanum products, Coumarins, Quinolines, Vetiver oil, etc. and it finds some use in Leather, Moss or dry Ambre types. Galbanum products offer good company with distinctly dry-green notes in "Miss Dior" type fragrance, etc.

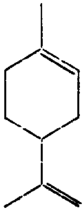
The material is rarely offered under its proper chemical name, but it is marketed in the shape of perfume specialties or bases in which it may be an important odor component, although only minute by volume.

Prod.: from *iso*-Propylpyrogallol.

68-481;
see also: 68-473;

## 1074: DIPENTENE

*1*-Methyl-*4*-*iso*-propenyl-*1*-cyclohexene.
"Dycom" (Newport Div. of Velsicol, U.S.A.)
Cinene.
*dl*-Limonene.
*racemic*-Limonene (*i*-Limonene).
Commercial grade Dipentene may contain about 75% Dipentene, the balance being higher and lower boiling Turpentine hydrocarbons.



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.84.
B.P. 178° C.

Flammable, but its vapors do not form explosive mixtures with air under normal working temperature conditions.

Insoluble in water, almost insoluble in Propylene glycol and Glycerin, soluble in alcohol, miscible with most oils.

Commercial grade Dipentene contains 8-10% Terpinene, some *para*-Cymene and other impurities. *para*-Cymene in particular, being much more volatile, influences the odor of commercial Dipentene to a considerable degree: gassy-piney, at times almost kerosene-like.

Pure Dipentene smells pleasantly citrusy, almost Lemon-like, fresh and sweet.

Good grade Dipentene is very useful in perfumery as a "lift" in citrusy fragrances, and in the reconstruction of many essential oils (Bergamot, Lime, Lemon, etc.).

Ordinary, commercial grades are used in masking odors for industrial purposes, and in certain types of detergent or heavy-duty household fragrances.

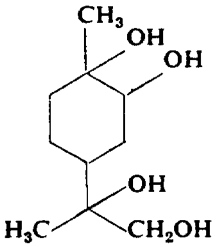
Prod.: by isolation (fractionation) from American Pine oil, and from rosin oils. It also appears as a by-product in the manufacture of Terpineol (particularly in Europe) and in various synthetic products made from *alpha*-Pinene or Turpentine oil.

Also: by thermal polymerisation of Isoprene.

26-592; 31-7; 44-806; 87-45; 100-609;
B-V-137; 67-401; 67-507;

## 1075: DIPENTENE TETROL

*para*-Menthane-*1,2,8,9*-tetrol.



$C_{10}H_{20}O_4 = 204.27$

Colorless, slightly viscous liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Very mild, sweet, balsamic-floral odor of moderate tenacity.

The commercial product – rarely available – shows considerable variations in odor, according to age and origin. Interested consumers generally prepare their own material.

The title material has found some use in perfumery, together with Limonene diol, the corresponding dihydric alcohol. The materials have a blending and sweetening effect, are very inexpensive, and the raw material for their production plentifully available in the U.S.A.

Prod.: by oxidation of Dipentene (or Limonene) with Potassium permanganate or with Hydrogen peroxide using an Osmium tetroxide catalyst.

87-69;

## 1076: DI-beta-PENTENYL TETRASULFIDE

$CH_3CH_2CH{=}CH{-}CH_2{-}S{-}S{-}S{-}S{-}$
$CH_2{-}CH{=}CH{-}CH_2{-}CH_3$

$C_{10}H_{18}S_4 = 266.52$

Pale yellowish liquid. Sp.Gr. 1.10.

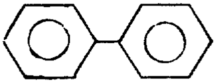
Powerful and penetrating, but sweet and in extreme dilution pleasant-green foliage odor. The concentrated material is difficult to evaluate because of its repulsively strong odor. Upon dilution the herbaceous character seems to increase, finally turning greener, earthy-vegetable-like just before the point of minimum perceptible.

This material has found some use in the reconstruction of certain essential oils, and as a trace ingredient in topnote compositions for perfumes or perfume bases. It is also used to a minor degree in flavor compositions, mainly in meat and vegetable (soup) flavors.

90-830; 11-5;

## 1077: DIPHENYL

Biphenyl.
Phenyl benzol.
Xenene.



$C_{12}H_{10} = 154.21$

Colorless crystals, M.P. 71° C. B.P. 256° C. Sp.Gr. 0.99 (liquid).

Insoluble in water, 10% soluble in alcohol, miscible with most oils.

Peculiar odor, gassy-green, remotely reminiscent of Geranium, but overall mild and rather nondescript, choking in high concentration. Sometimes described as "metallic" odor.

Has been suggested for use in soap and powder perfumes as a fixative for Rose and Geranium type fragrances.

This chemical is primarily marketed for use as a fungus growth inhibitor to impregnate the wrapping paper in which Citrus fruits are packed for shipping or export.

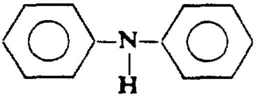
Diphenyl is toxic and acts as a depressant upon the human CNS.

Prod.:

1) by pyrolytic dehydrogenation of Benzene.
2) by isolation from coal tar.

4-47; 26-526; 68-1033; 100-380; 86-48; B-V-576; 1-396;

## 1078: DIPHENYLAMINE



$C_{12}H_{11}N = 169.23$

White crystals. M.P. 54° C. B.P. 302° C. Sp.Gr. 1.16 (liquid).

Flammable when heated. Discolors in daylight. Insoluble in water, 40% soluble in alcohol, miscible with most oils.

The pure material has a faint, sweet, floral odor, but most commercial lots display a "chemical" note, varying from gassy to fishy.

The author believes that this material is not used as such in perfumes or flavors, but it is occasionally used as an antioxidant or stabilizer in various perfume chemicals. It is therefore important that a high-grade material is used.

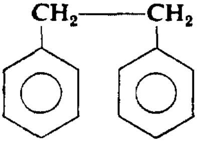
It is irritating to human mucous membranes, but it is considered less toxic than Aniline.

Produced from Aniline plus Aniline hydrochloride at 260° C.

68-181; 26-526; 100-380; B-XII-174;

## 1079: DIPHENYL ETHANE

*1,2*-Diphenyl ethane.
Dibenzyl.



$C_{14}H_{14} = 182.27$

Colorless prismatic crystals. M.P. 52° C. B.P. 284° C. Sp.Gr. 0.98 (liquid).

Insoluble in water, soluble in alcohol and oils.

Mild, rather sweet odor of metallic-green Geranium type, not very natural, but quite pleasant in dilution. Tenacious.

Has been suggested for use in soap and detergent perfumes, partly as a modifier for Diphenyl methane, which is somewhat harsher, but also more powerful, partly as a fixative in general for Rose-type or Geranium-type low-cost fragrances.

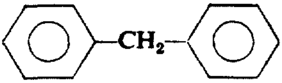
Prod.:

1) from Benzyl chloride plus Sodium.
2) from Dichloroethylene (or *beta*-Phenylethyl chloride) by condensation with Benzol, using Aluminium chloride in a Friedel-Crafts reaction.

1-400; 4-42; 26-528; 30-358; 68-1137; 86-48; B-V-605;
See also: Methyl-diphenylmethane (2007).

## 1080: DIPHENYL METHANE

Ditane.
Benzyl benzene.



$C_{13}H_{12} = 168.24$

Colorless prismatic crystals or colorless liquid, solidifying in the cold, melting at 27° C. Sp.Gr. 1.00 (liquid). B.P. 262° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Harsh Geranium-leaf, Orange-blossom type odor. More pleasant and less "metallic" when diluted.

Used in perfume compositions for its power and moderate fixative effect. It is an inexpensive odorant, which in skilled hands may turn out quite attractive notes. However, its odor type limits its application to rather few fragrance types.

Apart from Geranium, Rose and various floral types, it can be used in New Mown Hay or Fougères substituting for Acetanisole in part, and it blends quite well with fruity notes such as Peach and Raspberry.

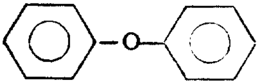
Prod.:

1) from Benzyl chloride plus Benzol with Aluminium chloride (Friedel-Crafts synthesis).
2) from Methylene chloride plus Benzol with Aluminum amalgam.

1-399; 4-47; 5-8; 26-528; 31-6; 31-11; 68-1055; 86-49; 95-81; 96-57; 100-382; B-V-588; 106-140; 103-277;

## 1081: DIPHENYL OXIDE

Diphenyl ether.
Phenylether.
"Geranium crystals".



$C_{12}H_{10}O = 170.21$

Colorless, long crystal needles, or colorless oily liquid, solidifying in the cold, melting at 28° C.

Sp.Gr. 1.07 (liquid). B.P. 252° C.

Very slightly soluble in water, soluble in alcohol and oils.

Harsh floral-green, metallic Geranium type odor. The crystals appear to emit a much milder odor than the liquid material, and it is only in actual use that one can truly estimate and evaluate the strength of this material, often underestimated by the inexperienced perfumer.

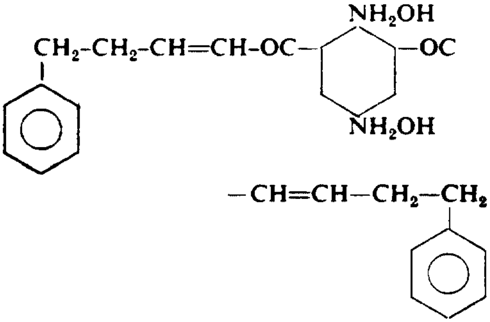
Often used in combination with Diphenyl methane or Diphenyl ethane, it finds a place in various types of fragrance for detergents and soaps, and many other household products. It is not confined exclusively to Geranium and Rose types, since Fougeres, New Mown Hay and Hyacinth, to mention a few, can benefit from this chemical. Like many other low-cost perfume chemicals, it is often an interesting tool in the hands of a skilled perfumer with audacity and imagination and an urge to use materials in an "unconventional" way.

Prod.: from Bromobenzene plus Potassium phenoxide heated with Copper at 220° C.

1-436; 4-47; 26-528; 5-227; 68-429; 86-48; 95-114; B-VI-146;

## 1082: DI-5-PHENYL-2-PENTENOYL PIPERAZONE, (A) and DI-5-PHENYL-3-PENTENOYL PIPERAZONE (B)

The structure below describes a theoretical picture of Di-*5*-phenyl-*2*-pentenoyl piperazonium salt (A).



$C_{26}H_{34}N_2O_4 = 438.57$

White crystalline powder. M.P. 153° C. (A) and 127° C. (B).

Soluble in water, poorly soluble in alcohol, insoluble in most oils.

Practically odorless. Powerful pungent taste resembling the biting pungency of Pepper.

The two title isomers have been manufactured in search of pungent principles in Black Pepper or derivatives which could be manufactured synthetically. However, since the Black Pepper components have been synthetically manufactured for a number of years and are commercially available, there is probably little future in the subject salts. Piperine, Piperidine, Chavicine and several hydrolytic products of Piperine have been made commercially available and a "reconstituted Pepper" can be prepared from such materials in acceptable quality.

Prod.: from Piperazine and 5-Phenylpentenoic acid (or its chloride).

50-219;

## 1083: DI-5-PHENYL-n-VALEROYL PIPERAZONE

The product originally produced was
Di-*5*-phenyl-*n*-valeroyl piperazonium salt.
For theoretical structure, see previous monograph.

$C_{26}H_{38}N_2O_4$ = 442.61

White crystalline powder. M.P. 120° C.

Soluble in water, somewhat soluble in alcohol, insoluble in most oils.

Pungent peppery taste and burning mouthfeel. Practically odorless.

See notes under previous monograph.

This material was developed in search of proof that the Piperazines had (or had not) a burning, peppery taste and biting mouthfeel. Earlier statements that the Piperazines were pungent, were contradicted by experiments carried out as early as the 1940's.

The title material has, in the author's opinion, lost its importance and has only academic interest today.

Prod.: from Piperazine and 5-Phenylvaleric acid (or chloride).

50-219;

## 1084: DIPROPIONYL

*3,4*-Hexandione.
(An isomer of Acetyl butyryl).

$(C_2H_5)CO—CO(C_2H_5)$

$C_6H_{10}O_2$ = 119.15

Yellow liquid. B.P. 130° C. Sp.Gr. 0.94.

Very slightly soluble in water, soluble in alcohol and oils, fairly soluble in Propylene glycol.

Pungent buttery odor, not as diffusive or penetrating as Diacetyl, but resembling that.

The taste is not as sweet as that of Diacetyl, and not as powerful.

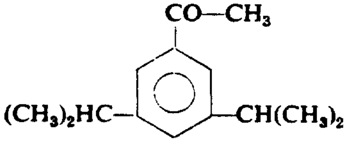
Has been suggested for use in flavor compositions as a modifier for Diacetyl, Acetyl butyryl, etc. However, it does not seem to offer any interesting notes which are not found in the conventional ketones.

Prod.: by oxidation of Ethyl propyl ketone with Selenium oxide.

66-721; 86-49;

## 1085: DI-iso-PROPYL ACETOPHENONE

The commercial product is mainly:
*3,5*-Di-*iso*-propyl-*1*-acetylbenzene.
(Traces of isomers are present).



$C_{14}H_{20}O$ = 204.31

Colorless oily liquid. B.P. 255° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, herbaceous-winey odor, often described as resembling that of Ambrette seed. The author finds that it is more like that of refined Labdanum extracts (absolutes). Fair to good tenacity.

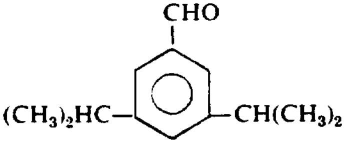
This material, developed in a research program based upon interesting results from mono-alkyl substituted Acetophenones (the *para-iso*-Propylacetophenone has a Cumin-Orris character), has been suggested for use in perfume compositions of floral or sweet woody character. The title material is rarely offered under its proper chemical name, but enters as component of several perfume bases and specialties.

The odor similarity to Ambrette seed should be considered with some restriction, since any perfumer who uses Ambrette seed absolute, will have great doubts about using the subject chemical as part substitute. However, it may play the same role in Ambrette bases as the lower alkyl-substituted Acetophenones do for Mimosa: lend power at low cost and, with proper blending and creative technique, produce an acceptable fragrance in low cost functional products.

31-83; 86-46;
see also U.S. Pat. (1930) 1776154;

## 1086: DI-iso-PROPYL BENZALDEHYDE

"Ambriol" (Agfa).
The commercial product consists mainly of:
*3,5*-Di-*iso*-propylbenzaldehyde.
Literature has also used the word:
Benzaldehyde di-*iso*-propylacetal as the chemical name for "Ambriol", but the author believes that the title name is correct.



$C_{13}H_{18}O = 190.29$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, slightly woody odor, often described as resembling that of Ambrette seed. Moderate to good tenacity.

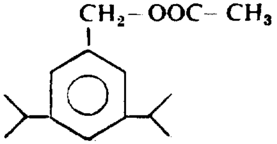
This aldehyde was marketed as a specialty at a time when very few chemicals with this odor type were available. Its very poor stability and high tendency of oxidation are drawbacks that speak very much against the extensive use of the material today, when many materials of this odor type are available.

When properly incorporated in a well-created base, this aldehyde can lend very interesting and powerful effects, e. g. as a modifier for the conventional Methylnonylacetaldehyde effect. It also blends well with Labdanum products. Orris and Ionones, Cyclamen aldehyde, etc.

4-7; 86-46;
see also: *2,4*-Di-*tertiary*-butyl-*5*-(and-*6*-)-methoxybenzaldehyde (Musk odors).

## 1087: DI-iso-PROPYL BENZYLACETATE

The commercial product consisted mainly of *3,5*-Di-*iso*-propyl benzylacetate.



$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Powerful fruity-floral odor of Jasmin type. Fair to good tenacity.

This ester was developed in search of new and powerful Jasmin odorants to substitute or modify Benzylacetate.

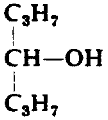
It has rarely been offered under its proper chemical name, but has entered several specialties as major or chief component of Jasmin bases or floral bases.

Newer alkyl substituted Benzylacetates have been prepared and have become more important. The title material may be considered as practically obsolete.

See also *2,4*-Dimethyl benzylacetate.

## 1088: DIPROPYL CARBINOL

*4*-Heptanol.
A secondary Heptyl alcohol.



$$\begin{array}{l} C_3H_7 \\ | \\ CH{-}OH \\ | \\ C_3H_7 \end{array}$$

$C_7H_{16}O = 116.21$

Colorless liquid. Sp.Gr. 0.82. B.P. 155° C.

Insoluble in water, soluble in alcohol and oils.

Pungent and rather harsh, but in proper dilution floral and pleasantly green odor.

This secondary alcohol has been suggested for use in perfume compositions to support floral notes, mainly with Terpineol and other low-cost ingredients for masking odors and industrial fragrances.

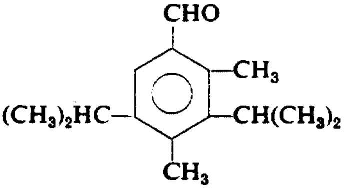
It finds only very limited use, and it requires very rich fixation in order to perform satisfactorily. Its low cost has probably supported its use in certain types of perfume.

Prod. by hydrogenation of Dipropylketone (or Di-*iso*-propylketone).

160-1028;

## 1089: DI-iso-PROPYL DIMETHYL BENZALDEHYDE

*2,4*-Dimethyl-*3,5*-di-*iso*-propylbenzaldehyde.



$C_{13}H_{20}O = 192.30$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, floral-musky odor of good tenacity. Often described as resembling the odor of Ambrette seed. The author would conditionally agree on this description, but not if the meaning is "Ambrette seed oil". The odor of the title aldehyde is far too dry to be compared to that of the Ambrette seed oil, which is characterized by rich vinous-floral sweetness and enormous tenacity in delicate musky notes.

However, this aldehyde did find some application in perfumery, until more effective and more readily available floral-musk type chemicals were developed.

The material came out of research on Nitromusks, and it is related to the better known "Ambral" which is mentioned in this work under the title: *2,4*-Di-*tertiary*-butyl-*5*-methoxybenzaldehyde.

It is furthermore interesting to observe the similatiry to
*3,5*-Di-*tertiary*-butyl benzaldehyde, which has a strong musk odor, and
*2,4*-Di-*iso*-propylbenzaldehyde, which has a mild, sweet musky odor.

## 1090: DIPROPYL KETONE

Di-*n*-propyl ketone.
*4*-Heptanone.
Butyrone.
NOTE: The Di-*iso*-propyl ketone is also known commercially as "Butyrone".

$CH_3(CH_2)_2{-}CO{-}(CH_2)_2CH_3$

$C_7H_{14}O = 114.19$

Colorless liquid. Sp.Gr. 0.82. B.P. 144° C.

0.5 % soluble in water, miscible with alcohol and oils.

Powerful and diffusive ethereal-fruity, pungent odor, in dilution reminiscent of Pineapple-Strawberry.

Fruity, Strawberry type flavor, but not really sweet, and lacks naturalness.

Rarely, if ever, used in perfumery.

Finds some use in flavor compositions, mainly in "Tutti-frutti" types, Strawberry, Pineapple-mix flavors, etc.

The concentration in the finished product will normally be about 1 to 30 ppm.

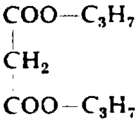
Prod.: by hydrolysis of *n*-Hept-*3*-yne.

G.R.A.S. F.E.M.A. No.2546.

4-27; 26-532; 66-517; B-I-699;

## 1091: DIPROPYL MALONATE

Propyl malonate.



$$\begin{array}{l} COO-C_3H_7 \\ | \\ CH_2 \\ | \\ COO-C_3H_7 \end{array}$$

$C_9H_{16}O_4 = 188.23$

Colorless liquid. Sp.Gr. 1.01. B.P. 229° C.

Very slightly soluble in water, soluble in alcohol and oils.

Ethereal, fruity-winey odor, mild and comparatively weak.

Has been suggested for use in flavor compositions, e. g. Brandy, Rum, Tutti-frutti, etc.

However, the taste is rather mild and uncharacteristic, and the material remains an occasional blender/modifier, rarely used.

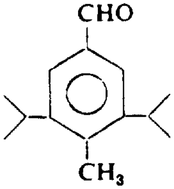
Prod.: by hydrolysis of Cyanoacetic acid with propylalcoholic hydrogen chloride.

4-121; 66-962; 163-66;

## 1092: DI-iso-PROPYL METHYLBENZALDEHYDE

*3,5*-Di-*iso*-propyl-*4*-tolylaldehyde.

"Homo-Ambriol".



$C_{14}H_{20}O = 204.31$

Although the title aldehyde has been described in perfumery literature as having an Ambregris-type of odor, the author has his doubts that this information could be correct.

*2,4*-Di-*iso*-propylphenylacetaldehyde, which is an empirical isomer, has been described as having a Musk-like odor. That aldehyde is used in the synthesis of Ethyl-*2,4*-di-*iso*-propylphenylglycidate (see that monograph) which has an Ambregris-type odor. It is most conceivable that confusion with the said aldehyde and the title material exists.

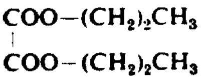
Yet, with repeated references in recent literature, the title aldehyde deserves mention as a chemical with possible application as an Ambrette-seed type odorant. It is described as having a slightly sweeter odor and being more tenacious than its lower homologue, described in this work under the name: Di-*iso*-propylbenzaldehyde.

It is interesting to note that Di-*iso*-propylacetophenone has a similar odor type.

4-261;

## 1093: DIPROPYL OXALATE

Di-*n*-propyl oxalate.



$$\begin{array}{l} COO-(CH_2)_2CH_3 \\ | \\ COO-(CH_2)_2CH_3 \end{array}$$

$C_8H_{14}O_4 = 174.20$

Colorless liquid. Sp.Gr. 1.02. B.P. 215° C. (-*iso*-propylester: 189° C.).

Very slightly soluble in water, miscible with alcohol and most flavor oils.

Very mild, winey-green odor with a tart-fruity-note.

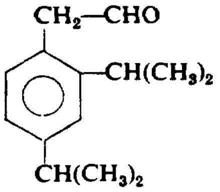
The taste of this chemical is somewhat astringent, green-fruity, yet mild.

Has been suggested for use in flavor compositions, particularly in Gooseberry, Blackcurrant, Rhubarb, Guava, etc., all of which are rather difficult flavor problems.

Prod. by direct esterification of *n*-Propanol with Oxalic acid, using azeotropic conditions.

4-122; 66-956;

## 1094: 2,4-DI-iso-PROPYL PHENYLACETALDEHYDE



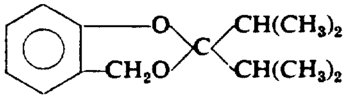
$C_{14}H_{20}O = 204.31$

This chemical, which is described as having a Musk type odor and possible application in perfumery is, to the author's knowledge, not offered commercially under its proper chemical name.

5-326; 86-46;

## 1095: DI-iso-PROPYL SALIGENIN KETAL

*ortho*-Hydroxybenzylalcohol di-*iso*-propylketal.
Salicylalcohol di-*iso*-propylketal.



$C_{14}H_{20}O_2 = 220.31$

This chemical is described as having a Rose-Honey type odor. It represents one member of a long series of research chemicals developed – when presumably Agfa in the 1920's – studied various derivatives of Phenols, etc.

Ketals were prepared from Monophenols, Diphenols, Phenol-alcohols, etc.

The author believes that the subject chemical still remains on the research shelf.

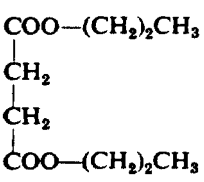
Prod.: by condensation of *ortho*-Hydroxybenzylalcohol with Di-*iso*-propylketone.

NOTE: It is interesting to compare the structure and odor of this chemical to that of Ethyl-*ortho*-methoxy benzylether (see monograph).

31-119;

## 1096: DIPROPYL SUCCINATE

*n*-Propyl succinate.



$$\begin{array}{l} COO{-}(CH_2)_2CH_3 \\ | \\ CH_2 \\ | \\ CH_2 \\ | \\ COO{-}(CH_2)_2CH_3 \end{array}$$

$C_{10}H_{18}O_4 = 202.25$

Colorless liquid. Sp.Gr. 1.00. B.P. 251° C.

Very slightly soluble in water, miscible with alcohol and oils.

Very mild, fruity-winey odor.

Somewhat astringent, mildly green, berry-like taste.

Used in flavor compositions for imitation Blackcurrant, certain types of Cherry, and other berry flavors.

This material is NOT listed in the G.R.A.S. list of the U.S. Federal Register.

Prod.: by direct esterification of *n*-Propanol with Succinic acid e. g. under azeotropic conditions.

4-122; 66-970;

## 1097: DISODIUM GUANYLATE

Disodium-5′-guanylate.

Constitutes approximately 44% of the commercial product known as "Mertaste" (Merck & Co.) – the balance (56%) being Disodium inosinate (see next).

Also known as "Ribotide" (TAKEDA Chem. Ind. - Japan) which is a similar mixture.
One component acts as a synergist upon the other with respect to meat flavor enhancing.

$C_{10}H_{12}N_5Na_2O_8P = 407.2$

The commercial product is a white crystalline powder, containing about 8% moisture.

The above mentioned mixture 44/56 is used at the concentration of approximately 50 to 150 ppm in finished consumer products to enhance meat flavors, soup flavors, etc., particularly in canned and spray-dried foods.

This chemical individually, and the above mentioned mixture will react synergistically with Monosodium glumate as meat flavor enhancers.

Info.: Merck & Co. data sheets 1964.
158-261 ff.

## 1098: DISODIUM INOSINATE

Disodium-5′-inosinate.
Constitutes approximately 56% of the commercial product known as "Mertaste" (Merck & Co.) – the balance being Disodium guanylate.
"Ribotide" (Takeda).
One component acts as a synergist upon the other with respect to meat flavor enhancing.

$C_{10}H_{11}N_4Na_2O_8P = 392.2$ (anhydrous)*.

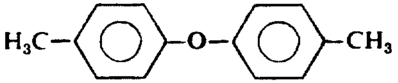
* Commercial product is a white crystalline powder, containing 7½ Mol. $H_2O$ per Mol. of Disodium inosinate. This is equivalent to about 27% water.

See notes under Disodium guanylate. The inosinate also reacts as a synergist with Monosodium glumate.

Info.: Merck & Co. data sheets 1964.
158-261 ff.
(also: Takeda Chemical Industries, Japan).

## 1099: DITOLYL ETHER

*para*-Cresyloxide.
*para*-Cresyl ether.



$C_{14}H_{14}O = 198.27$

White or colorless flaky or leafy crystals.

Almost insoluble in water, soluble in alcohol, miscible with most perfume oils.

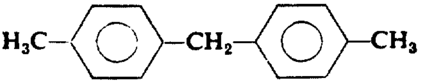
Mild, green-rosy, somewhat woody odor of great tenacity.

Suggested for use in soap and detergent perfumes, partly as a fixative, partly as a background note in Rose, Geranium, Lavender, New Mown Hay, Fougère and many other perfume types. It is sufficiently mild, not harsh, that it can be utilized in a great variety of fragrance types.

Originally marketed as a fragrance material by Dow Chemical Co., Aromatic Division, it has not always been commercially available since the original producer discontinued manufacturing the item.

The Di-*ortho*-cresyloxide is still used in England and elsewhere in Europe. See that monograph.

## 1100: DI-para-TOLYLMETHANE



$C_{15}H_{16} = 196.29$

Colorless oily liquid or colorless crystalline mass. M.P. 23° C. B.P. 291° C.

Woody-rosy, rather faint odor with a remote resemblance to Geraniol (low-grade).

Suggested for use in perfumery for soap perfumes of Sweet Pea type, Rose, Geranium, sweet-woody fragrances, etc.

Not a very common chemical, rarely offered commercially from the usual suppliers of fragrance chemicals.

Prod.: from Benzylchloride and Toluene with Zinc dust catalyst.

4-42; 7-161; 31-6; 31-11; 34-912; 37-170; 86-49;

## 1101: DODECA-2,4-DIEN-1-AL

Nonenyl acrolein.

$CH_3(CH_2)_6CH{=}CH{-}CH{=}CH{-}CHO$

$C_{12}H_{20}O = 180.19$

Almost colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Very powerful, Grapefruit-Orange type odor, most attractive in concentrations below 0.1 %.

A fairly recent addition to the perfumer's shelf, this aldehyde provides new notes in the almost trivial "aldehydic" topnote theme.

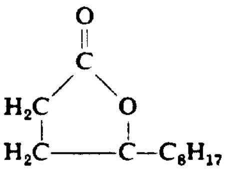
It introduces very fine notes in Citrus oils, particularly Grapefruit and Bitter Orange, and it blends well with the conventional alifatic aldehydes in woody, mossy or citrusy compositions. As a trace ingredient in topnote compositions for floral fragrances, it has also good possibilities.

Prod.: by double addition of Acetaldehyde to Octanal, or by condensation of Crotonaldehyde with Octanal.

Sample: Compagnie Parento, Inc.

## 1102: gamma-DODECALACTONE

Dodecanolide-*1,4*.
*gamma-n*-Octyl-*gamma-n*-butyrolactone.



$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid. Sp.Gr. 0.94. B.P. 258° C.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Fatty-peachy, somewhat musky odor, fattier than Undecanolide.

Finds some use in perfume compositions for fatty-fruity topnotes and long tenacity e. g. in heavy floral fragrances. It is also used in combination with newer synthetic musks to produce exceptional tenacity and lasting sweetness in powdery and in floral types.

Used in flavor compositions, mainly in Butter, Butterscotch, Coconut, Tutti-frutti, Maple, Nut, Peach, Pineapple, etc.

Concentration is normally mere traces in the functional product.

Prod.:

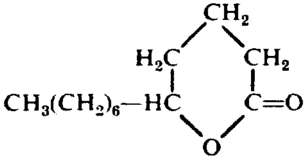
1) from *4*-Hydroxy dodecanoic acid by lactonization.
2) from Methyl acrylate plus Octanol with a catalyst.

G.R.A.S. F.E.M.A. No.2400.

31-174; 156-229;

## 1103: delta-DODECALACTONE

*n*-Heptyl-*delta*-valerolactone.
5-Hydroxydodecanoic acid, *delta*-lactone.



$C_{12}H_{22}O_2 = 198.31$

Colorless or very pale straw-colored, viscous liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Powerful, fresh-fruity, oily odor of good tenacity. Fruitier than the odor of *gamma*-Dodecalactone, and not as musky.

The taste is Pear-Peach-Plum-like at suitable dilution, which is 2 to 5 ppm or even less.

A comparatively new Lactone of interesting effect in aldehydic perfumes, heavy florals (Gardenia-Tuberose, etc.) and in general for new notes.

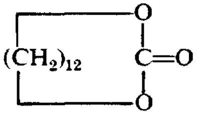
It is used in flavor compositions, in mere traces, for imitation Butter and Pear, and in various fruit complexes.

G.R.A.S. F.E.M.A. No.2401.

Prod.: from 5-Hydroxydodecanoic acid by lactonization.

Samples and data: Soda Aromatic Co., Japan.

## 1104: DODECAMETHYLENE CARBONATE



$C_{13}H_{24}O_3 = 228.34$

A macrocyclic musk of little more than academic interest. The two-Methylene-higher members of this series have more pronounced and powerful musky odors, but none are as powerful and truly musky as the isomer series of Oxahexadecanolides.

The author believes that subject material is more or less obsolete as a perfume raw material.

30-272; 31-127;
See also: Tetradecamethylene carboxylate – and Oxahexadecanolide.

## 1105: DODECANAL

Dodecylic aldehyde.
Aldehyde C-12 Lauric.
Lauric aldehyde.
Lauryl aldehyde.

$CH_3(CH_2)_{10}CHO$

$C_{12}H_{24}O = 184.31$

Colorless oily liquid, solidifying in the cold, melting again at 44° C. (or at 11° C.).
B.P. 249° C.

Almost insoluble in water, soluble in alcohol, oils, Propylene glycol, Mineral oil, but not in Glycerin.

Sweet, waxy-herbaceous, very fresh and clean-floral odor (Lily-Violet-like in dilution) with a faint, balsamic undertone. The odor is often referred to as "fresh-laundry-odor", but it is only pleasant in extreme dilutions. The concentrated material has a rather fatty-waxy odor.

Polymerizes easily, solidifies, but may be de-polymerized by heating. The material suffers however, by intermittant heating and cooling and should be kept at a steady room temperature.

It is one of the most extensively used alifatic aldehydes in perfumery. Its versatility is probably its greatest asset: from Pine to Violet, from detergent perfumes to luxury lotion fragrances it finds its way into a multitude of fragrance types: Pine, Pine needle, floral, "modern", Citrus complexes, Chypres, etc.

The aldehyde finds also use in flavor compositions for imitation Butter, Banana, Caramel, Honey, Lemon, Lime, Orange, Tangerine, as well as in Neroli florals and various fruit complexes.

The concentration of this aldehyde in the finished consumer product is normally about 1 to 3 ppm, but may be as high as 100 ppm in chewing gum.

FCC-1964-849. G.R.A.S.
F.E.M.A. No.2615.
Prod.: by catalytic dehydrogenation of Dodecanol (Lauryl alcohol).

4-47; 5-86; 6-86; 26-590; 31-49; 31-55; 41-34; 77-203; 35-1073; 89-32; 106-38; 156-18; B-I-714; 140-159;

## 1106: DODECANAL DIMETHYLACETAL

Aldehyde C-12,DMA.
Lauric aldehyde dimethylacetal.
*12,12*-Dimethoxydodecane.

$C_{11}H_{23}—CH(OCH_3)_2$

$C_{14}H_{30}O_2 = 230.39$

Colorless liquid. Poorly soluble in water, soluble in alcohol and oils.

Very faint, fresh-green and slightly oily odor with a fruity-waxy undertone.

Has been suggested for use in perfumery, but its lack of power and the fact that the parent aldehyde is quite stable under normal concentration and chemical conditions in the functional products, has made the acetal more or less superfluous.

It has found a little use in flavors, mainly in Honey types where its soft waxy notes can be utilized. However, it should be remembered that this acetal, like most others, is unstable in acid media – a condition which is prevalent in many flavored products.

Prod. from Dodecanal and Methanol under dry hydrogen chloride.

4-80;

## 1107: DODECANOIC ACID

Laurostearic acid. (technical, commercial name).
Lauric acid.
Dodecoic acid.

$CH_3(CH_2)_{10}COOH$

$C_{12}H_{24}O_2 = 200.32$

White crystalline powder. M.P. 44° C.
Sp.Gr. 0.86 (liquid).

Insoluble in water, soluble 50% in alcohol, miscible with most oils.

The purified grade of this chemical has very little odor, but a lower grade, commercially known as Laurostearic acid, has a fatty-waxy odor, yet overall a refreshing note.

Dodecanoic acid is used in Butter flavors and in certain Citrus flavor types, mainly in Lemon.

The concentration used may vary from 2 to 40 ppm, calculated upon the finished consumer product.

Prod.: from Coconut oil by saponification.
G.R.A.S. F.E.M.A. No.2614.

86-82; 90-99; 100-599;

## 1108: DODECANOL

Dodecyl alcohol (*n-primary*).
Lauric alcohol.
Lauryl alcohol.
Undecyl carbinol.
*l*-Dodecanol.
Alcohol C-12.
Tuberol (old name).
Tuberyl alcohol (old name).
Lorol # 5 (commercial grade).
Lorol # 9 (about 70% Dodecanol).
Lorol # 11 (about 80% Dodecanol).

$CH_3(CH_2)_{10}CH_2OH$

$C_{12}H_{26}O = 186.33$

Colorless oily liquid, or white or colorless leafy crystals or microcrystalline mass, melting at 24° C. B.P. 259° C. Sp.Gr. 0.84 (liquid).

Insoluble in water and Glycerin, soluble in alcohol, Propylene glycol, Mineral oil and most perfume and flavor oils.

Very mild, oily-fatty, slightly waxy, but fresh and remotely "soapy" odor. Pure grades have a certain similarity to fragrance notes in Mimosa, Cassie, Tuberose in the waxy-green floralness.

Commercial grade (most common: Lorol No. 5) is a mixture of alifatic alcohols with an even number of Carbon atoms: C-10, C-12, C-14, C-16, C-18.

Finds extensive use as a solvent/diluent/blender in low-cost perfumes, often accompanying the corresponding aldehyde. It lends soft notes to Pine, floral bases, "modern" and aldehydic complexes, fresh and citrusy types, etc. and it is well liked in detergent fragrances.

In flavors, it finds use in Citrus types, Coconut bases, floral types, fruit complexes, Honey imitations, etc.

Concentration is normally only 1 to 8 ppm in the finished product, but may run as high as 15 to 30 ppm in chewing gum.

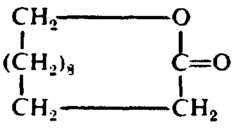
FCC-1964-847; G.R.A.S.
F.E.M.A. No.2617.

Prod.: from saponified Coconut oil. The acids are purified by fractional distillation, esterified, and the purified Ethylester is reduced to Dodecanol with Sodium ethylate.

26-534; 41-27; 61-54; 31-16; 86-477; 100-390; 106-31; B-I-428; 77-172; 35-1073; 140-125;

## 1109: 1:12-DODECANOLIDE

Dodecyllactone-*1:12*.
"Cyclododecalactone".



$C_{12}H_{22}O_2 = 198.31$

Colorless viscous liquid, solidifying in the cold, melting at about 2 to 3° C.
B.P. approximately 220° C. Sp.Gr. 0.98.

Practically insoluble in water, soluble in alcohol and oils.

Mild, woody-musky odor of moderate to good tenacity.

This lactone, developed in a series of experiments aiming at interesting macrocyclic musks, represents the lowest member of this series that can be said to have at least some interest as a fragrance material. Its odor is not purely musky, its tenacity leaves much to be desired, and its effect is in no way comparable to that of the higher members, particularly Pentadecanolide (3 members higher homologue).

It was particularly interesting to note that the chemicals, from which these lower members of the macrocyclic musk family could be synthesized are found in waxy materials from a number of common Conifers, e. g. Juniper, Sabina, etc.

Prod.: by lactonization of *omega*-Hydroxylauric acid (also known as Sabinic acid).

4-47; 66-802; 86-49; 159-439;

## 1110: n-DODECEN-2-AL

2-Dodecenal.
3-Nonyl acrolein.
*trans*-2-Dodecen-1-al.

$CH_3(CH_2)_8CH{=}CH{-}CHO$

$C_{12}H_{22}O = 182.31$

Colorless oily liquid. B.P. 272° C.

Insoluble in water, soluble in alcohol and oils.

Powerful citrusy odor, unpleasant gassy, choking at high concentration, but interestingly natural, Orange-Mandarin-like in extreme dilution.

Taste is Mandarin-like at concentrations below 2 ppm.

Could find some use in perfumery, but it takes quite some experience and skill to fully utilize the character of this aldehyde without having its unpleasant notes dominating the composition.

Finds use in flavor compositions, mainly in Orange and Mandarin imitation flavors. The concentration is always mere traces.

G.R.A.S. F.E.M.A. No.2402.

Prod.: by condensation of Acetaldehyde with Decanal. Also from *alpha*-Bromolauric acid via its Ethylester and alcohol.

89-49; 156-26;
Sample: Compagnie Parento, Inc. (U.S.A.).

## 1111: DODECENOL

Dodecylenic alcohol.
Two isomers have been produced for perfumes and flavors:

A) *omega*-Dodecenol – the most interesting, and
B) 3-Nonyl allylalcohol, occuring in Nature, but of limited use.

A) $CH_2{=}CH(CH_2)_9CH_2OH$
B) $CH_3(CH_2)_8CH{=}CH{-}CH_2OH$

$C_{12}H_{24}O = 184.32$

A) White waxy-crystalline mass, melting at 60° C. to a colorless oily liquid. Insoluble in water, soluble in alcohol and oils. Orange-waxy, sweet-floral, fresh and somewhat fruity odor.

Could find use in perfume compositions as part of new and interesting topnote compositions with fresh-fruity, citrusy, or delicately floral character. The odor type blends well with Muguet, certain types of Rose, Peony, etc., as well as with Neroli. In compositions with the conventional alifatic aldehydes, it can introduce new and very pleasant nuances.

Prod.:
A) from Dodecamethylene glycol.
B) from *alpha*-Bromolauric acid via Dodecenoic acid and its Ethylester to the alcohol.

## 1112: DODECENYL PROPIONATE

*omega*-Dodecenyl propionate.

$CH_2{=}CH(CH_2)_9CH_2{-}OOC{-}C_2H_5$

$C_{15}H_{28}O = 224.39$

Colorless, slightly oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, floral-musky, slightly oily odor with notes reminiscent of Orris absolute and Ambrette seed oil.

A very interesting perfume chemical with many possible uses. Its power places it among new and pleasant topnote items, while its odor type make it extremely versatile in general application from floral to Ambre or woody fragrance types.

It is particularly interesting to note that this chemical is characterized by a floral-musky and Ambrette-seed note, and that the chemical formula shows 15 Carbon atoms and 28 Hydrogens, exactly like some of the newest and most promising macrocyclic musks, some of which have the formula $C_{15}H_{28}O_3$. It is commonly agreed, that an increase in Oxygen atoms generally enhances the power of the odor.

There are very few perfume (or flavor) materials with an Ambrette-seed like odor, and the availability of any such chemical should be most welcome.

Prod.: by esterification of *omega*-Dodecenol.

## 1113: n-DODECYL ACETATE

Lauryl acetate.
Acetate C-12.
Dodecanyl acetate.
Lauric acetate.

$CH_3(CH_2)_{11}—OOC—CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.
B.P. 257° C.

Refreshing, waxy-fruity odor with citrusy note.

Useful in perfume formulations, particularly as a topnote ingredient – in spite of its high boiling point. In fact, the performance of odor, shown by this chemical, is quite remarkable. A lasting odor from the very topnote throughout the various stages of evaporation of the fragrance. However, it needs blending with other materials to become more attractive, especially Citrus oils, light, fruity notes or light woody notes. It will also impart a pleasant freshness to sophisticated Pine fragrances, and in Carnation bases.

Dodecyl acetate is also used in flavor compositions for imitation Butter, Lemon, Orange, Peach, Pineapple, etc. and in various meat flavor bases.

The concentration in the finished product will normally be about 1 to 6 ppm.

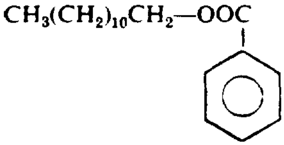
G.R.A.S. F.E.M.A. No.2616.

Prod. by direct esterification of Lauryl alcohol with Acetic acid (azeotropic conditions) or with Acetic anhydride.

41-18; 43-504; 44-806; B-II-135; 26-534; 103-100; 140-135;

## 1114: DODECYL BENZOATE

Lauryl benzoate.



$CH_3(CH_2)_{10}CH_2—OOC—C_6H_5$

$C_{19}H_{30}O_2 = 290.45$

Although subject material has been marketed from time to time, the author believes that it has very little to offer to the creative perfumer.

A truly pure grade of Lauryl benzoate has very little odor, and the odor has very little character.

The material serves occasionally as a fixative/blender in floral or Oriental fragrances, and it has a pleasant influence upon Labdanum products, often taking the sharpness out of these.

Prod.: by direct esterification, using azeotropic conditions.

## 1115: DODECYL BUTYRATE

Lauryl butyrate.

$CH_3(CH_2)_{11}—OOC(CH_2)_2CH_3$

$C_{16}H_{32}O_2 = 256.43$

Colorless liquid, insoluble in water, soluble in alcohol and oils. B.P. 315° C.
Sp.Gr. 0.89.

Very mild, oily-rancid odor, not exactly pleasant, and not characteristic of any common natural odor.

Has been suggested as modifier for lower Dodecyl esters in mild floral bases, Ambre types, etc. but this ester seem to have very little to offer with respect to unusual notes or power, etc.

Prod.: by direct esterification of Dodecanol with *n*-Butyric acid using azeotropic conditions.

35-1075;

## 1116: DODECYL-iso-BUTYRATE

Lauryl-*iso*-butyrate.

$CH_3(CH_2)_{11}—OOC—CH(CH_3)_2$

$C_{16}H_{32}O_2 = 256.43$

Colorless oily liquid. Sp.Gr. 0.88
B.P. 299° C.

Insoluble in water, soluble in alcohol and oils.

Not more interesting than the *n*-Butylester.

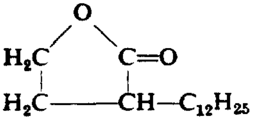
Could find a little use in perfumery in certain floral bases, in Ambre-like topnotes, as a support to winey-floral-musky topnotes, etc.

Very rarely offered commercially.

Prod. by direct esterification of Dodecyl alcohol with *iso*-Butyric acid preferably using azeotropic condition.

## 1117: alpha-DODECYL-gamma-BUTYROLACTONE

"Stearolactone".



$C_{16}H_{30}O_2 = 254.42$

Colorless to very pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol, almost insoluble in Glycerin.

Musky, Coconut-like, fatty odor of great tenacity.

This material is rarely offered commercially. The lactone is interesting by the fact that its empirical formula is the same as that of Hexadecanolide (Dihydro ambrettolide). The Butyrolactone ring introduces the fruity character and bars the musky notes from becoming dominating or truly musky.

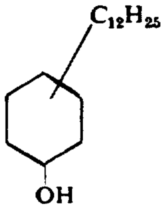
Finds a little use in perfume compositions as a modifier for Undecanolide in modern musky-fruity fragrance types, etc.

Its taste is not sweet enough to make an interesting flavor chemical out of it.

31-170; 159-418;

## 1118: DODECYL CYCLOHEXANOL

(Presumably a mixture of isomers).



$C_{18}H_{36}O = 268.49$

A number of alkyl-substituted Cyclohexanols have been prepared and some of them were found to be interesting perfume chemicals.

A few have survived the first many years of tests and doubts, and the subject material is one material that has reached beyond the research shelf.

However, it does not seem that the perfumers have taken this chemical to their hearts, and it may slowly disappear from the market.

One manufacturer suggested it for use in perfumery, particularly for soaps as a floral blender, interesting for woody, orrisy and mildly floral compositions.

Prod.: by catalytic reduction of Dodecyl phenol.

31-25;

## 1119: DODECYL FORMATE

Lauryl formate.

$CH_3(CH_2)_{10}—CH_2—OOC—H$

$C_{13}H_{26}O_2 = 214.35$

Colorless, oily liquid. B.P. 280° C.
Sp.Gr. 0.88.

Insoluble in water, soluble in alcohol and oils.

Mild, green-fruity, somewhat floral, Honeysuckle-type odor, also resembling Linden-blossom and Lily.

Finds a little use in perfumery as a modifier for the Acetate, and in itself for its fresher, greener note and greater power.

It imparts quite interesting and pleasant notes in Tuberose and Narcissus, Lily, Hyacinth bases, etc. and it blends excellently with the conventional alifatic aldehydes.

Prod.: by esterification of Dodecanol with Formic acid and Acetic anhydride.

35-1075;

## 1120: DODECYL MERCAPTAN

Lauryl mercaptan.
*1*-Dodecane thiol.

$C_{12}H_{25}—SH$

$C_{12}H_{26}S = 202.41$

Pale yellowish or almost colorless, mobile liquid.

Practically insoluble in water, soluble in alcohol and oils.

The undiluted material has an irritating effect upon the human mucous membranes and skin.

In extreme dilution the material shows a pleasant herbaceous, mildly oily-green odor, reminiscent of vegetables and leaves.

Has been suggested for use in perfume bases and in artificial essential oils. Its use is very limited.

Prod.: from Dodecyl bromide plus Potassium sulfhydrate in cold alcoholic solution.

## 1121: DODECYL NITRILE

The name is a misnomer, since it actually refers to Undecyl cyanide, and should be called: Dodecanoic nitrile.

$C_{11}H_{23}—C{\equiv}N$

$C_{12}H_{23}N = 181.32$

Colorless oily liquid, solidifying in the cold, melting at 4° C. B.P. 252° C.

Very slightly soluble in water, soluble in alcohol and oils.

Warm, woody and slightly fatty-aldehydic odor with a spicy undertone.

This Nitrile is another member of a large family of Nitriles, developed since the early 1950's, when a systematic research program was undertaken by Antoine Chiris Co. under Dr. Georges Igolen in Grasse, France. (See also MYRISTIC NITRILE).

It became evident, that many Nitriles had odor types similar to those of the corresponding Aldehydes. And since certain Aldehydes caused trouble in perfumery under alkaline conditions, there was an interest in any such material which would be stable under alkaline conditions and have the odor qualities of the Aldehydes.

It is common practise to name the Nitrile by the name of the acid which can be formed by acid hydrolysis of the Nitrile. The Nitrile with 12 Carbon atoms (total) will therefore be DODECANOIC NITRILE or LAURIC NITRILE.

It has been suggested for use in perfume compositions as a powerful fragrance-diffusing agent in soap perfumes, and as a modifier in topnote compositions where aldehydes, woodnotes or green notes are predominant. However, it does not perform like Dodecanal (Aldehyde C-12) and should not be considered as a replacement for that aldehyde.

Prod.: (many methods) e. g.: from Undecyl bromide and Potassium cyanide.

66-601;

## 1122: DODECYL PROPIONATE

Lauryl propionate.

$CH_3(CH_2)_{10}CH_2—OOC—C_2H_5$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Fruity-winey odor, reminiscent of Ambrette seed oil with a fatty-Pineapple-like and slightly earthy undertone.

Finds some use in perfume compositions, mainly as part of a topnote complex. It blends well with the alifatic aldehydes, and lends tenacity and a pleasant muskiness to delicately floral notes, it softens citrusnotes and offers a natural, petal-like note to many floral fragrances.

With the lower alifatic esters, it can build pleasant winey complexes for other types of topnote bases.

Prod.: by direct esterification of Dodecanol with Propionic acid under azeotropic conditions, or with Propionic anhydride.

7-237; 7-406; 35-1075; 43-622;

## 1123: DODECYL VALERATE

Lauryl pentanoate.

$CH_3(CH_2)_{11}—OOC(CH_2)_3CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless liquid. Sp.Gr. 0.86. B.P. 320° C.

Insoluble in water, soluble in alcohol and oils.

Oily-fruity, faintly floral odor with some resemblance to that of unripe Apples, but with an almost nauseatingly sweet-oily note.

However, being quite mild overall, this chemical can find use in topnote compositions as part of the fixative section. It blends well with Cognac oil, alifatic aldehydes, terpeneless Citrus oils, Undecalactone, etc. – quite a versatile material.

Very rarely offered commercially.

Prod.: by direct esterification of Dodecanol with *n*-Valeric acid under azeotropic conditions.

35-1074;

## 1124: DODECYL-iso-VALERATE

Lauryl-*iso*-valerate.

$CH_3(CH_2)_{11}—OOC—CH_2—CH(CH_3)_2$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid. Sp.Gr. 0.85.
B.P. 302° C.

Insoluble in water-, soluble in alcohol and oils.

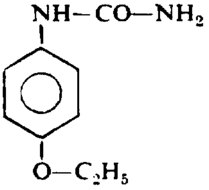
Oily-fruity, fresh-Apple-like odor with a rather heavy undertone. Overall weak and not very natural.

Has been suggested for use in perfumery as a replacement for the *n*-Valerate, which is less stable. However, the general opinion is that the *n*-Valerate is somewhat more natural in character.

Prod.: by direct esterification of Dodecanol with *iso*-Valeric acid under azeotropic conditions.

## 1125: DULCIN

*para*-Phenethole carbamide.
"Sucrol".
*para*-Phenethyl urea.
*para*-Ethoxy phenyl urea.



$C_9H_{12}N_2O_2 = 180.21$

Colorless and odorless, needlelike crystals or white crystalline powder. M.P. 174° C.

Soluble 0.1% in cold water, 2% in boiling water, 4% in alcohol, insoluble in most oils.

Intensely sweet taste, approximately 250 times sweeter than cane sugar when compared in dilution.

A "classic" among the non-caloric sweetening agents for human food preparations, Dulcin is no longer important.

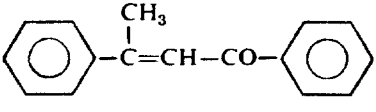
The chemical breaks down in the human organism yielding among other products *para*-Aminophenol – which is considered toxic. Dulcin is therefore NOT permitted for use as a sweetener in food. (FDA-1950).

Prod.: from *para*-Phenetidine plus Carbonyl chloride, followed by treatment with Ammonia.

1-474; 30-335; 100-393; 68-455;
See also: *N*-Methyl phenethyl carbamide.

## 1126: DYPNONE

Di-hypnone.
*1,3*-Diphenyl-*2*-buten-*1*-one.
*beta*-Methyl chalkone.
*beta*-Methyl phenyl styryl ketone.



$C_{16}H_{14}O = 222.29$

Yellowish liquid. Sp.Gr. 1.11. B.P. 345° C. (decomposes).

Insoluble in water, soluble in alcohol and oils.

Very faint, but tenacious, sweet, slightly buttery odor.

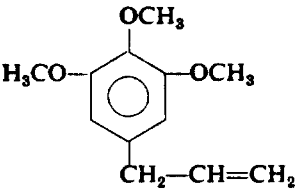
Although this chemical is not truly a perfume or flavor material, it is briefly mentioned because it enters as an active ingredient in cosmetic preparations, and it does slightly influence the odor of a perfume added to that preparation. It acts as a sunscreening agent.

Prod.: by condensation of 2 Mol. Acetophenone, using Aluminium chloride as a catalyst in boiling Xylene.

31-84; 68-1183; 86-50; 100-395;

## 1127: ELEMICINE

*4*-Allyl-*1,2,6*-trimethoxybenzene.



$C_{12}H_{16}O_3 = 208.26$

Colorless to pale straw-colored, viscous liquid. Sp.Gr. 1.06. B.P. 246° C.

Very faint, sweet, somewhat woody-floral odor with a spicy undertone.

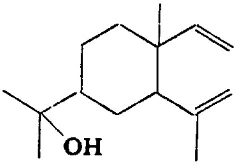
The material as such is rarely used in perfumery, but fractions of essential oils, rich in Elemicine, are used in soap perfumes, low-cost fragrances for detergents and other household products, mostly as a fixative and blender in mild florals, citrusy or woody fragrance types.

Prod.:

1) by isolation from Elemi oil (high-boiling fractions).
2) from Dimethylpyrogallol plus Allyl bromide, via *2,6*-Dimethyl pyrogallol allylether. This is heated in a Claisen-rearrangement reaction to yield *4*-Hydroxy-*3,5*-dimethoxy allylbenzene. The latter is methylated to yield Elemicine.
3) From Eugenol via *5*-Hydroxyeugenol.

17-53; 65-534; 68-978; 90-482;

## 1128: ELEMOL



$C_{15}H_{26}O = 222.37$

Colorless or white crystals, melting at 52° C. Sp.Gr. (liquid) 0.92. B.P. 254° C.

Very faint, sweet-woody odor with an almost floral undertone.

Has been suggested for use in perfumery, but the pure material is not a common commercial article. Fractions from certain essential oils, rich in Elemol, are used as fixatives, blenders or modifiers in low cost soap perfumes, detergent fragrances and other household product fragrances.

Elemol-fractions blend very well with Amyris oil, Guaiacwood oil, Geraniol, Amyl salicylate, Terpineol, etc. rounding off the roughness of chemicals, and sweetening other materials. Overall, however, it is of very little odor value, and it is always a problem to use a fraction of a certain essential oil or a byproduct from same. A problem of availability.

Prod.: by isolation from Java-type Citronella oil, usually by boration of the high-boiling fractions.

Also from high-boiling fractions of Elemi oil.

4-48; 7-164; 65-262; 67-676; 88-250;

## 1129: ELEMYL ACETATE

$C_{15}H_{25}—OOC—CH_3$
(structure - see Elemol)

$C_{17}H_{28}O_2 = 264.41$

Pale straw-colored, viscous liquid.

Insoluble in water, soluble in alcohol, miscible with most oils.

Sweet, slightly fruity-citrusy and very tenacious odor.

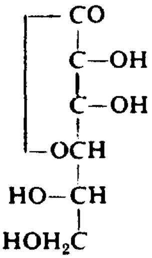
Has been suggested for use in perfume compositions, mainly soap perfumes, etc., but the material is not available in the quantities needed for such purposes.

Prod.: by Acetylation of Elemol in a hydrocarbon diluent.

Elemyl acetate resembles Eudesmyl acetate in structure and odor.

## 1130: ERYTHORBIC ACID

D-Arabascorbic acid.
*iso*-Ascorbic acid.
Also known under a number of trade names.



$C_6H_8O_6 = 176.13$

White granular crystals. M.P. 168-171° C.

40% soluble in water. Soluble in alcohol, slightly soluble in Glycerin and Propylene glycol.

Practically odorless.

Clean acidulous taste, resembling that of Citric acid, but somewhat milder.

Finds use as an antioxidant in food products, and is mentioned only because it does have a taste and will influence the flavor of the product.

Normal concentration in the finished product is 20 to 500 ppm. With respect to Vitamin C effect, it is 20 times weaker than Ascorbic acid.

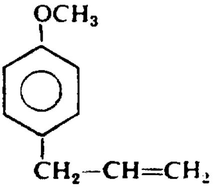
Prod.: from D-Fructose.

F.E.M.A. No.2410. G.R.A.S.

66-1276; 100-571; 140-145;

## 1131: ESTRAGOLE

Methyl chavicol.
*iso*-Anethole.
*para*-Allyl anisole.
Esdragol.
*para*-Methoxy allyl benzene.
Chavicyl methylether.
(Commercial grade contains approximately 90% Estragole*).



$C_{10}H_{12}O = 148.21$

Colorless, slightly oily liquid. Sp.Gr. 0.97. B.P. 216° C.

Almost insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Sweet-herbaceous Anise-Fennel type odor. Much more herbaceous than Anethole, and not as intensely sweet.

The taste is not nearly as sweet as that of Anethole, and not as "clean" or singular. More warm-herbaceous, complex.

Useful in perfume compositions for herbaceous Fougères, Lavenders, Chypres, Pine fragrances, etc. and particularly in soap perfumes. Its "candy"-like character limits its use considerably in perfume compositions, but in modest concentration it can have good influence upon many floral fragrances as well, Lilac, Appleblossom, Heliotrope, etc.

More widely used in flavor compositions, particularly in seasonings, dressings, condiments and meat flavors. As a modifier for Anethole it finds use in Licorice flavorings, and in smaller amounts in Spice blends, fruit flavors, Liqueurs, etc.

Concentration may be about 40 ppm in baked goods, and up to 150 ppm in chewing gum.

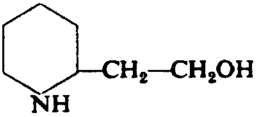
Prod.: from fractions of American wood turpentine oil, by isolation. A synthesis from Allyl bromide and *para*-Methoxyphenylmagnesium bromide has little practical importance.

G.R.A.S. F.E.M.A. No.2411.

17-44; 17-54; 17-271; 26-536; 34-679; 68-969; 72-35; 90-426; 95-118; 96-101; 100-417; 106-142; B-VI-571; 104-225; 77-199; 140-169; *) (Arizona Chemical Co.).

## 1132: 2-ETHANOL PIPERIDINE

*2-alpha*-Hydroxyethyl hexahydropyridine.



$C_7H_{15}NO = 129.21$

Almost colorless or pale straw-colored, slightly viscous liquid. Very slightly soluble in water, soluble in alcohol and oils.

Mild, sweet, nauseating-floral, warm-herbaceous odor of moderate tenacity. The commercial grades may vary in odor quality, and there are unacceptable types among the less pure materials.

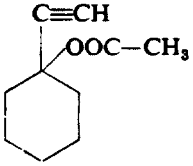
The title material has been suggested for use in perfume compositions, mainly as a "heavy" note in the more pungent-floral types: Jasmin, Gardenia, Tuberose, etc. It has also an interesting effect upon Civet and Castoreum, mellowing the animal notes into a more pleasant theme. With Benzyl phenylacetate and similar materials, it is occasionally used for sweet tobacco-like notes in certain perfume bases.

Prod.: from *2-alpha*-Pyridylethanol by hydrogenation.

69-550;
Sample: Reilly Tar and Chemical Co. (U.S.A.)

## 1133: ETHINYL CYCLOHEXYLACETATE

*1*-Ethynyl cyclohexan-*1*-ylacetate.



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, somewhat green, and in high concentration rather gassy odor of moderate to poor tenacity. In dilution quite pleasant and more natural-herbaceous.

This rare ester has been used in perfume compositions for its powerful herbaceous effect, mainly in conjunction with Lavender, Lavandin and with Cyclohexanyl derivatives, woody notes, Ionones, Amylsalicylate, etc.

It is not marketed under its proper chemical name, and it is no longer regularly available, indicating that it may have lost its importance in perfumery.

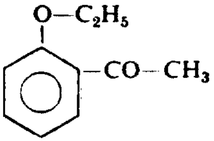
Prod.: from Cyclohexanone with Sodium Acetylide in ether or similar inert solvent, followed by esterification.

The title ester also occurs in one process as an intermediate in the making of Cyclohexylidene acetaldehyde.

67-173; 67-191;

## 1134: ortho-ETHOXY ACETOPHENONE

*ortho*-Acetyl phenethole.
*1*-Ethoxy-*2*-acetylbenzene.
"Homo-*ortho*-acetanisole".



$C_{10}H_{12}O_2 = 164.21$

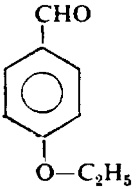
This chemical has been described in literature as a material with potential use in perfumery. Its odor is described as "Jasmin-like".

In view of its structure, it is possible, however, to predict that its odor is not typical of any important part of the Jasmin picture, but the material is most conceivably a good fixative with rich sweetness, tenacity and possessing floral as well as herbaceous notes.

31-83;

## 1135: para-ETHOXY BENZALDEHYDE

"Ethyl aubepine" (misleading, old name).
"Homoanisaldehyde".



$C_9H_{10}O_2 = 150.18$

Colorless liquid. Solidifies in the cold, melting at 14° C. B.P. 249° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, floral and somewhat herbaceous odor of good tenacity. Milder than Anisaldehyde, more floral, less herbaceous, but overall not quite as powerful.

Finds a little use in perfume compositions where the harsher notes of Anisaldehyde prevents extensive use of that material, in general as a floralizer with fair stability in soap and good performance in room sprays, etc.

Traces of this aldehyde are used in Vanilla and fruit flavor compositions, partly as a sweetener, partly as a modifier for Heliotropine, Anisalcohol, Vanillin and other sweeteners.

G.R.A.S. F.E.M.A. No.2413.

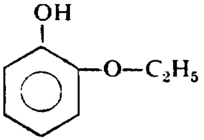
Prod.: by Ethylation of *para*-Hydroxybenzaldehyde. This aldehyde, which is very important as an intermediate in the manufacture of many naturally occurring flavor chemicals can be prepared from Phenol plus Hydrocyanic acid plus Hydrochloric acid.

The Ethylation of the hydroxyaldehyde is carried out using Aluminium chloride as a catalyst.

68-744;

## 1136: ortho-ETHOXYPHENOL

Catechol monoethylether.
Ethyl catechol.
Ethacol.
Guaethol. (Do NOT confuse with Ethyl guaiacol).
"Homoguaiacol".
*ortho*-Hydroxy phenethol.



$C_8H_{10}O_2 = 138.17$

Colorless or very pale straw-colored liquid. Solidifies in the cold, melts at 28° C.
B.P. 217° C.

Soluble in aqueous alkali. Very slightly soluble in water, soluble in alcohol and oils. Extremely powerful, diffusive and intensely medicinal-phenolic, yet sweet and spicy-warm, remotely Vanilla-like odor.

In dilutions below 2 ppm its taste is sweet and remotely Vanilla-like.

This powerful odorant can be used in perfume compositions to emphasize "leather"-like odors, medicinal odors, or smoky-tobacco-like odors. It is an interesting modifier for the Quinolines, and it has found use recently in many types of household products where a "medicated" odor is desirable or in line with the function of the product. Traces of this phenol can be used in the heavy floral fragrance types. It blends well with Castoreum, Styrax, Labdanum, etc.

In flavors, it can be used to increase the power of Vanilla formulations and to reduce the overly sweet effect of Vanillin-Ethylvanillin, and as a modifier for Propenyl guaethol.

Prod.: by Monoethylation of Catechol with Diethylsulfate in aqueous alkaline solution.

26-538; 68-467; B-VI-771;

## 1137: ETHYL ACETATE

Acetic ether.
"Vinegar naphta".

$CH_3—COO—C_2H_5$

$C_4H_8O_2 = 88.11$

Colorless, mobile liquid. B.P. 77° C.
Sp.Gr. 0.90.

Soluble 8% in water at room temperature, more in colder water. Water will dissolve 3.5% Ethylacetate.

Miscible with alcohol, Propylene glycol, Glycerin and oils.

Pleasant, ethereal-fruity, Brandy-like odor, somewhat nauseating in high concentration.

Fruity-sweet, ethereal taste when freshly diluted in water (Ethyl acetate is easily hydrolyzed in water, increasing the acidity).

The ester is highly flammable, its vapors form explosive mixtures with air at room temperature.

Only rarely used in perfume compositions, occasionally to make a topnote smell "aged" or more rounded-alcoholic, or to give a "lift" to Citrus notes or other light notes, etc.

The ester is probably one of the most used of all flavor chemicals by volume. It forms a major part of the imitation flavors of many berry-types, Banana, Grape, Pineapple, Peach, Lemon, Tutti-frutti, Whisky, Rum, Almond, Butterscotch, Creamsoda, Butter, Mint, Pear, Melon, Arak, etc. etc.

The concentration used in the finished product is usually rather high - up to 200 ppm in gelatins, puddings, etc. - and up to 1500 ppm in chewing gum.

It is interesting to note that concentration of the vapors in air higher than 400 ppm are considerered hazardous to the human respiratory system. However, it should be kept in mind, that the ester is decomposed extremely fast in the digestive system, and therefore probably more tolerable orally than by inhalation.

G.R.A.S. F.E.M.A. No.2414.

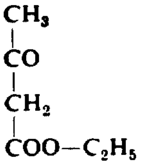
Prod.: from Ethyl alcohol and Acetic acid – usually in a multicolumnar distillation system, often taking advantage of low-cost, low-proof alcohol and low-concentration Acetic acid. It is extremely important that the ester is anhydrous ("absolute Ethyl acetate") for flavors and perfumes. Traces of Alcohol are not harmful to the effect of the ester.

26-538; 31-134; 43-500; 44-806; 77-181; 100-422; 90-195; B-II-125; 140-134;

30*

## 1138: ETHYL ACETOACETATE

Acetoacetic ester.
Ethyl acetyl acetate.
Ethyl-*3*-oxobutanoate.
Commercial product is a mixture of Keto- and -enol forms.



$CH_3—CO—CH_2—COO—C_2H_5$

$C_6H_{10}O_3 = 130.15$

Colorless liquid. Sp.Gr. 1.03. B.P. 181° C. 2.8% soluble in water, miscible with Alcohol, Propylene glycol and oils.

Ethereal-fruity, sweet and Rum-like odor. Sweet, fruity, somewhat "fermented-overripe" fruity taste in water.

Occasionally used in perfume compositions, mainly to support ethereal, winey, brandylike, fresh-citrusy and other light, non-floral topnotes. It has also been used to introduce an "aged" note to alcohol in alcoholic tinctures (lotions) of perfume compositions.

Finds wider use in flavor compositions, where its pleasant Rum-like taste can be utilized in almost any type of fruity and winey flavor: Apple, Apricot, Berry, Cherry, Peach, Whisky, Rum, Arak, Liqueurs, etc.

Concentration may be about 125 ppm in baked goods and up to 500 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2415.

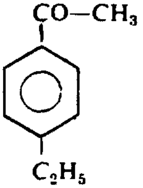
Prod.: by reduction of Ethyl acetate with Sodium Ethylate.

Ethyl acetoacetate is flammable but not hazardous. Flash point 50° C.

26-538; 31-134; 44-806; 77-192; 100-423; B-III-632; 140-149;

## 1139: para-ETHYL ACETOPHENONE

"Ethyl acetophenone".
*4*-Ethyl-*1*-acetylbenzene.



$C_{10}H_{12}O = 148.21$

Colorless liquid. Almost insoluble in water, soluble in alcohol, miscible with most oils.

Sweet, warm, somewhat pungent-floral odor with a herbaceous-balsamic undertone.

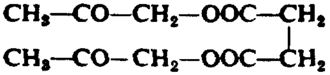
This material finds a little use in heavy floral compositions such as Ylang-Ylang, but also in non-floral fragrance types such as Ambre (it blends very well with Labdanum and Castoreum), or as a modifier in Mimosa-Cassie bases, New Mown Hay or tobacco-types, etc.

To control the pungency, it is useful to blend this ketone with Anisalcohol or its derivatives, Labdanum derivatives. Coumarin substances, etc. However, in certain heavy florals, the pungency is more or less desirable, and the ketone makes a pleasant variation of its lower homologue, Methyl acetophenone.

It is a comparatively rare chemical, offered from the manufacturers of "fine chemicals" rather from perfume chemical manufacturers.

Prod.: from *para*-Ethylphenol plus Acetylchloride with Aluminum chloride in an inert solvent (Friedel-Craft's reaction).

## 1140: ETHYL ACETOSUCCINATE



$$\begin{array}{l} CH_3-CO-CH_2-OOC-CH_2 \\ \qquad\qquad\qquad\qquad\qquad\quad | \\ CH_3-CO-CH_2-OOC-CH_2 \end{array}$$

$C_{10}H_{14}O_4 = 198.22$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Mild, caramellic-sweet, fruity-winey odor, reminiscent of "cooked" fruits.

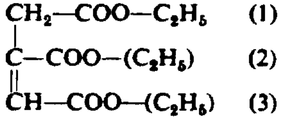
Sweet-fruity-winey-taste.

Occasionally used in flavor compositions for imitation Cherry, Peach, Plum, etc.

4-14;

## 1141: ETHYL ACONITATE

Ethyl-*2*-carboxyglutaconate.
Ethyl-*1*-propene-*1,2,3*-tricarboxylate.
An incompletely esterified product containing Mono-, Di- and Triethyl aconitate.



$$\begin{array}{lll} \textit{alpha:} & CH_2-COO-C_2H_5 & (1) \\ & | & \\ \textit{beta:} & C-COO-(C_2H_5) & (2) \\ & \| & \\ \textit{gamma:} & CH-COO-(C_2H_5) & (3) \end{array}$$

$C_8H_{10}O_6$ = 202.17 (*mono-*)
$C_{10}H_{14}O_6$ = 230.22 (*di-*)
$C_{12}H_{18}O_6$ = 258.28 (*tri-*)

Colorless liquid, heavier than water. Triethyl-ester: Sp.Gr. 1.06. B.P. 260° C.

Slightly soluble in water, soluble in alcohol and oils.

Sweet, slightly caramellic-fruity odor with a diffusive, winey note.

Finds some use in flavor compositions, mainly for Rum, Liqueur and various fruit flavors.

Concentration is normally about 60 ppm in baked goods.

G.R.A.S. F.E.M.A. No.2417.

Prod.: by catalytic dehydration of Citric acid, followed by esterification.

66-1152;

## 1142: ETHYL ACRYLATE

Ethyl propenoate.

$CH_2{=}CH{-}COO{-}C_2H_5$

$C_5H_8O_2$ = 100.12

Colorless liquid. Sp.Gr. 0.93. B.P. 101° C. (under polymerization).

1.5% soluble in water, miscible with alcohol and oils. Ethyl acrylate absorbs 1.5% water in aqueous media. It polymerizes easily under influence of air, heat or daylight. Fairly stable below 10° C. The polymer form is a transparent, resilient, odorless mass.

Acrid, penetrating odor, apparently very diffusive, yet surprisingly tenacious (possible polymerization on tissue, thereby augmented retention of odor.

Has occasionally found use in perfumery in the reconstruction of certain essential oils (Chamomile, etc.).

Finds some use in flavor compositions, mainly Pineapple and Raspberry, but also in fruit complexes, Liqueur flavorings, etc.

Concentration is usually limited to mere traces.

The ester is considered harmful – by some observers – to the human organism. It is a fact that it has lachrymatory effect in high concentration. (And so has Mustard oil, which is permitted).

G.R.A.S. (permitted in the U.S.A.) –
F.E.M.A. No.2418.

Prod.: By esterification of Acrylic acid, which can be obtained by a number of methods:

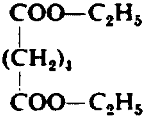
1) Dehydration of Ethylene cyanhydrin,
2) Oxidation of Acrolein,
3) Pyrolysis of Lactic acid acetate.

or – the Ethyl acrylate can be prepared directly from Acetylene, Carbon monoxide and Ethyl alcohol with Nickel catalyst.

26-540; 66-631; 90-220; 100-423; B-II-399;

## 1143: ETHYL ADIPATE

Diethyl adipate.
Diethyl hexanedioate.



$$\begin{array}{l} COO{-}C_2H_5 \\ | \\ (CH_2)_4 \\ | \\ COO{-}C_2H_5 \end{array}$$

$C_{10}H_{18}O_4$ = 202.25

Colorless liquid. Sp.Gr. 1.01. B.P. 245° C.

Soluble 0.4% in water, soluble in alcohol and oils.

Pleasant, rather powerful odor of vinous-oily-slightly fruity character.

Occasionally used in perfumery as a solvent/fixative.

Has been used in flavor compositions, mainly as a solvent, modifier, blender or fixative.

It has not much of a distinct character, but acts mostly softening, mellowing upon an established flavor composition.

Prod.: directly by esterification of Ethyl alcohol with Adipic acid, preferably under azeotropic conditions.

4-14; 26-496; 31-126; 66-982; 100-423; B-II-652;

# 1144: ETHYL ALCOHOL

Ethanol.
Alcohol.

$C_2H_5OH$

$C_2H_6O = 46.07$

Colorless mobile liquid. Sp.Gr. 0.79.
B.P. 78° C.

Miscible with water, Propylene glycol, Glycerin, perfume oils and most flavor oils, not with all hydrocarbons.

Commercial product is approximately 95% Ethylalcohol by volume or approximately 93% by weight. Anhydrous alcohol (so-called 200-proof) has little use in perfumes or flavors, but finds some use in aerosol solutions where water may be undesirable.

The odor is sweet-ethereal, mild (in view of its low boiling point which tempt us to expect a very diffusive odor) and it is perceptible in aqueous solutions down to about 12% alcohol and room temperature. The taste, however, is perceptible down to about 3% (maybe partly because of the fact that the solution is heated when taken into the mouth). Naturally, these figures are highly subjective and may fluctuate considerably from one observer to another.

Ethyl alcohol is used in perfumery almost exclusively as a solvent and for that purpose a denatured alcohol is required by law in most countries. Common denaturants are:
1% Diethyl phthalate or
5% Methanol or
10% Acetone or
5% Ethyl acetate or
0.12% tertiary Butanol plus a minute amount (0.027%) of Strychnine or Brucine, etc.

One percent Diethyl phthalate is a generally acceptable denaturant for perfume solutions, except for very weak solutions (containing only 1-2-4% of perfume oil) where the Diethylphthalate would act as a large, odor-depressing ingredient in the perfume oil, and constitute 20 to 50% of the oil-mixture.

The tertiary-Butanol-Strychnine denaturant is then the alternative. It has no measurable non-volatile matter, and does not act as an odor-depressant. It constitutes the purest and highest proof alcohol available for perfume solutions (92.3% by weight, 94,9% by volume), except for the special anhydrous alcohol (denatured) for aerosols.

It is generally agreed, that alcohol for perfume solutions should be reduced in strength – with water. At about 88% or lower alcohol strength, the odor of the ethyl alcohol itself seem to soften and is easily overcome by the smallest amounts of perfume oil. The lower limit of alcohol concentration is naturally set by the solubility of the perfume oil at low storage temperature.

Before using alcohol for perfume solutions, it should be carefully tested for odor purity. One of the most common "off-odors" is a sulfuric note of mercaptan type of note, usually perceptible at the dryout of the alcohol on a large smelling blotter after a few minutes. The water used for dilution should be pure, distilled or de-ionized water, passed a careful odor test.

The effect of the alcohol upon the perfume oil should only be that of a carrier. It should lift the perfume without contributing an odor of its own. Most odorless solvents do not lift, but actually depress the odor, and many "lifting" solvents have perceptible odors. Which makes ethyl alcohol well-nigh ideal.

Perfume solutions vary in strength from about 20% by weight down to less than 1%. The commercial product, classified as "perfume" is usually about 16% perfume oil and 84% diluted alcohol – by weight. Some countries use very conservative methods of measuring the oil and the alcohol (ounces to gallons, U.S. gallons or Imperial gallons, volume or weight etc. etc.) and the Revenue authorities still rely on volume measuring as a standard.

FLAVORS:

Ethyl alcohol for flavor use must be pure, undenatured alcohol. The strength of the alcohol is less important with flavors, since there is no problem of evaluating by odor or "lift". In fact, the alcohol for flavors is strictly a solvent, and used as sparingly as possible, often substituted by solvents of lower vapor pressure (Propylene glycol, etc.) but ethyl alcohol remains the universal solvent for flavor materials.

Natural alcohol is still used in many countries, however, there is but one manufacturer left in the U.S.A. The flavorist will often find that a good grade of Vodka is a purer ethyl alcohol than any ethyl alcohol from the manufacturers of synthetic alcohol. Vodka is too weak for general use as a solvent. The strongest alcoholic beverage commercially available is Rum, which is manufactured up to 75% by volume. At this strength, it is rarely consumed as such, but used for blending. Cognac comes out of the stills at about 56% by volume, but falls to about 46% during many years of ageing in wooden kegs that permit a certain amount of "breathing" of the alcohol, thereby incurring a loss of alcohol.

Wine is produced by fermentation of grapes and the fermentation stops at about 12-13% alcohol which is the upper limit at which the fungus can thrive. If wine is distilled ("gebrannt" in German language) a type of "Brandy" ("Branntwein") is produced with an alcohol content of 45 to 75. Alcohol produced by *fermentation* of starches or sugars other than grape sugar, are Whisky (from grain) Snaps (from potatoes), Rum (from sugar cane), Arak (from rice), Tequila (from agave juice) etc. etc.

The concentration of ethyl alcohol in finished consumer products is about 200 to 2000 ppm in beverages, icecream, chewing gum, candy, etc. and up to 450,000 ppm in alcoholic beverages (see above).

As an example, Rum has a perceptible flavor at the concentration of 5000 ppm in icecream. At that concentration it has an alcohol strength of only one-tenth of that of beer. Rum is therefore a comparatively powerful natural flavor material, in which the alcohol plays practically no role as a flavor contributor.

## USE IN FLAVORS:

Ethyl alcohol finds use in flavors also as an extraction solvent for natural materials and as an inhibitor against the growth of microorganisms. Solutions of more than 15% ethyl alcohol are normally safe against mold or fungus growth.

Diluted alcohol is used to prepare "tinctures" of terpeneless oils for flavor use. At 70% or often lower, down to 50% alcohol strength, the solvent will separate the terpenes and other hydrocarbon components from essential oils, etc. Citrus oils are therefore "washed" with diluted alcohol to produce flavor tinctures. The by-product is a "washed" citrus oil and it finds use in perfumery.

It is typical of alcoholic flavor extracts, however, that they are generally prepared with alcohol of lower strength than those used in perfumery. In fact, low-proof alcohol is often a better solvent for components of natural raw materials (for flavors) than highproof alcohol. This is particularly true for Vanilla extracts, etc.

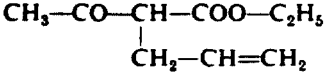
## ODOR QUALITY:

The importance of Ethyl alcohol in perfumes and flavors is unfortunately often underestimated. It should be kept in mind, that ethyl alcohol is the largest component in many functional fragrance products, its volume often amounting to 20, 50 or 100 times that of the fragrance materials total. Any odor impurity in ethyl alcohol may therefore be 100 times more dangerous than the total amount of odor impurities in all the fragrance materials that are dissolved in the alcohol. Evaluation of the odor quality of alcohol can be undertaken by smelling the alcohol in a large Brandy-glass ("snifter"), under slow, continuous dilution with pure, odorless water until the odor of the alcohol is no longer perceptible. Off-odors may occur before this point, but will often occur when there is no alcohol odor left.

Prod. (synth.) from: Acetylene via Acetaldehyde or other basic synthesis. Alcohol is on the American G.R.A.S. list, F.E.M.A. No. 2419.

26-540; 26-1785; 77-97; 100-28; B-I-292; 66-299; 77-167; 140-122;

## 1145: **ETHYL**-alpha-**ALLYL ACETOACETATE**



$$CH_3-CO-\underset{\displaystyle CH_2-CH=CH_2}{\underset{|}{CH}}-COO-C_2H_5$$

$C_9H_{14}O_3 = 170.21$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Fruity-green, sweet and ethereal odor, rather sharp and powerful in its initial note.

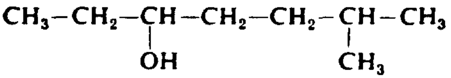
Has been suggested for use in perfume compositions, mainly as a topnote ingredient, a modifier for the conventional green and fruity materials. Its ethereal-winey character gives it a pleasant and generally acceptable odor, useful with Lavender, Lavandin, Citrus oils and Ambre bases. It gives interesting lift to Ylang Ylang and a few other powerful floral materials.

Originally appearing as a research chemical, developed from a program not related to perfumery, this chemical is no longer regularly available and may be an obsolete article.

(sample: U.S. Industr. Chem.).

## 1146: ETHYL-iso-AMYLCARBINOL

*6*-Methyl-*3*-heptanol.
*2*-Methyl-*5*-heptanol.



$$CH_3-CH_2-\underset{\underset{OH}{|}}{CH}-CH_2-CH_2-\underset{\underset{CH_3}{|}}{CH}-CH_3$$

$C_8H_{18}O = 130.23$

Colorless liquid.

Very slightly soluble in water, miscible with alcohol and oils.

Oily-floral, but rather harsh and unnatural odor of poor tenacity. Of the many commercially available Octanols, this is one of the least attractive from an odor point of view.

The material has been used in industrial perfumes as a masking agent, because it is very inexpensive, a good solvent, and abundantly available.

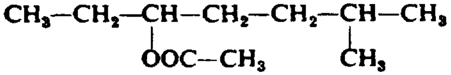
It also serves as a starting material for the manufacture of a number of other perfume chemicals.

Prod.: by hydrogenation of Ethyl-*iso*-amylketone.

See also monographs:
Octanol-*1*.
Methyl hexyl carbinol.
Methyl-*iso*-hexylcarbinol.
*3*-Octanol.

## 1147: ETHYL-iso-AMYL CARBINYLACETATE

*6*-Methylheptan-*3*-yl acetate.



$$CH_3-CH_2-\underset{\underset{OOC-CH_3}{|}}{CH}-CH_2-CH_2-\underset{\underset{CH_3}{|}}{CH}-CH_3$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Oily-fruity, fresh-herbaceous, but overall not very natural odor of moderate to poor tenacity. It is possible that the apparent harshness is due to impurities, since the title ester is usually derived from an industrial alcohol, manufactured in volume.

Apart from occasional use in low-cost masking odors for industrial and technical purposes, this ester has very little application in perfumery. It is generally considered too harsh for use with Lavender or other herbaceous fragrance materials.

See also monographs:
*n*-Octylacetate.
*2*-Octanyl acetate.
*3*-Octanyl acetate.

Prod.: by direct acetylation of the corresponding alcohol (see previous monograph).

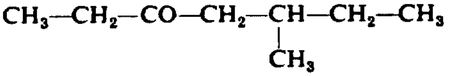
## 1148: ETHYL AMYL KETONE

Ethyl-*n*-amyl ketone.
*3*-Octanone.
E.A.K.

$CH_3—CH_2—CO—(CH_2)_4CH_3$

$C_8H_{16}O = 128.22$

NOTE: Ethyl amyl ketone (commercial, large-volume chemical) is *5*-Methyl-*3*-heptanone:



$$CH_3{-}CH_2{-}CO{-}CH_2{-}\underset{\displaystyle CH_3}{\underset{|}{CH}}{-}CH_2{-}CH_3$$

It is a colorless liquid. B.P. 160° C.

Slightly soluble in water.

It can NOT substitute *3*-Octanone in perfume compositions. Its odor is more flat-chemical, not as sweet-oily or herbaceous.

*3-Octanone:*

A colorless oily liquid, almost insoluble in water, soluble in alcohol and oils.

Sp.Gr. 0.82. B.P. 172° C.

Pungent, herbaceous-fruity, warm odor, somewhat spicy-buttery with distinct resemblance to the topnotes in Lavender oil.

Finds use in perfume compositions and – in particular – reconstruction of essential oils, mainly Lavender oil and Lavandin oil. It introduces great power and radiance in the sweet-herbaceous notes, and supports the buttery-earthy, characteristic topnotes of these oils.

The ketone is used in flavor compositions for imitation Cheese, Peach, Coffee, in spice blends and Citrus complexes, etc. Concentration in the finished product will normally be about 3 to 10 ppm.

G.R.A.S. F.E.M.A. No.2803.

Prod.:

1) by heating Propionic and Caproic acids over Thorium oxide,
2) by oxidation of Ethyl-*n*-amyl carbinol (*3*-Octanol).

– and several other methods.

4-14; 5-149; 26-540; 31-80; 45-402; 86-16; 89-170; 100-424; B-I-706; 140-165;

## 1149: ETHYL-iso-AMYL KETONE

*6*-Methylheptan-*3*-one.

$C_2H_5{-}CO{-}CH_2{-}CH_2{-}CH(CH_3)_2$

$C_8H_{16}O = 128.22$

Colorless oily liquid. Sp.Gr. 0.83.
B.P. 164° C.

Insoluble in water, soluble in alcohol and oils.

Weak, rather camphoraceous odor with less emphasis on the herbaceous notes, and not overall "warm" – as compared to Ethyl-*n*-amyl ketone.

See also NOTE – under Ethyl-*n*-amyl ketone.

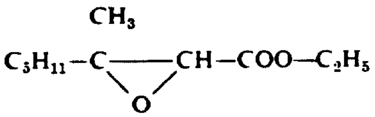
The Ethyl-*iso*-amyl ketone can not substitute the normal ketone, and it is only mentioned to emphasize the importance of the specific and correct chemical. There is a marked difference in the odor of the various isomers of this ketone.

The subject chemical is of little use in perfumery.

26-540; 31-80; B-I-706;

## 1150: ETHYL AMYL METHYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3*-methyloctanoate.
Amylmethylglycidic acid, ethylester.



$C_{11}H_{20}O_3 = 200.28$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Winey-sweet odor of Grape- and Berry-like character. Fair to good tenacity. Sweet, slightly fruity taste of Apple- and Berry type.

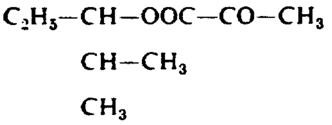
This glycidic ester is very rarely offered under its proper chemical name, and the author believes that it is rarely used at all.

It has been suggested for use in flavor compositions where it is said to be capable of introducing pleasant natural "fermentation" type notes in Grape, Apple, Berry and other imitation flavors where green-winey notes are desirable.

Prod.: from Methyl-*n*-amylketone plus Ethylmonochloroacetate plus Sodium methylate.

## 1151: ETHYL-iso-AMYLPYRUVATE

*2-iso*-Propylbutanol pyruvate.



$C_2H_5—CH—OOC—CO—CH_3$; $CH—CH_3$; $CH_3$

$C_{10}H_{18}O_3 = 186.25$

Colorless liquid. Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Fresh-winey, sweet and fruity, but also "tart" odor of moderate to poor tenacity.

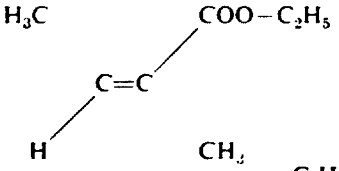
Tart-fruity, but in suitable dilution quite sweet taste, reminiscent of certain notes in Blackcurrant and other berries.

This ester has been suggested for use in flavor compositions for imitation Berry, Apple, Wine and in various fruit complexes.

Prod.: From *2-iso*-Propylbutanol-*1* by esterification with Pyruvic acid.

## 1152: ETHYL ANGELATE

Ethyl-*cis-2*-methyl crotonate.
Ethyl-*cis*-methylbutenoate.
Ethyl-*cis-2,3*-dimethyl acrylate.



$C_7H_{12}O_2 = 128.17$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.

Powerful and diffusive, warm-herbaceous

FLAVORS:

odor, sweet and winey with a caramellic undertone.

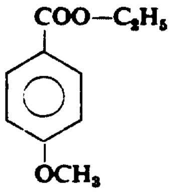
The ester has been suggested for use in various perfume bases, mainly herbaceous-warm bases, such as Chamomile. However, the high diffusiveness of this ester makes it a difficult item to control in a perfume composition where its initial power is of almost acrylic character.

Higher esters of Angelic and Tiglic acids are used more commonly in perfumery.

Prod.: by direct esterification of the alcohol with Angelic acid. Commercial Angelic acid usually contains considerable amounts of Tiglic acid.

## 1153: ETHYL ANISATE

*para*-Methoxy ethylbenzoate.
Ethyl-*para*-methoxybenzoate.



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid. Solidifies in the cold, melts at 8° C. Sp.Gr. 1.10. B.P. 270° C.

Insoluble in water, slightly soluble in Propylene glycol, miscible with alcohol and oils.

Sweet-floral, anisic-Fennel-like, mild odor with resemblance to Chervil, Hawthorn flowers, Anise and Fennel.

Useful in perfume compositions for certain floral bases:

Lilac, Appleblossom, Carnation, Ylang-

It is sweet without being candy-like, Anise seed like.

It is floral in a discrete way, suitable for Lilac, Acacia, Mimosa, etc.

The ester finds use in flavor compositions for many types of berry, Liqueur, fruit complexes, Grape, Licorice and Anise flavorings, Rum, Vanilla, Almond, etc.

A separate use is that in toothpaste and mouthwash flavors.

Concentration in finished products is about 5 to 7 ppm (in edible products) and somewhat higher in oral preparations.

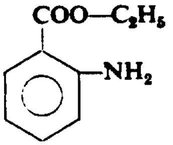
Prod.: by direct esterification of Ethyl alcohol with Anisic acid under azeotropic conditions. The acid is usually made from Anethole.

G.R.A.S. F.E.M.A. No.2420.

4-14; 26-540; 43-501; 44-680; 86-16;

## 1154: ETHYL ANTHRANILATE

Ethyl-*ortho*-aminobenzoate.
*2*-Amino ethylbenzoate.



$C_9H_{11}NO_2 = 165.20$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol. Sp.Gr. 1.12. M.P. 13° C. B.P. 267° C.

Sweet-fruity, grape-like odor, milder and less harsh than the Methyl ester.

Finds a little use in perfumery, but the Methylester is generally preferred because of its greater power.

Ethyl anthranilate is used in flavor compositions, particularly in Berry flavors, Grape, Mandarin, Orange, Peach, Raisin, in fruit complexes and in various floral compositions, such as Neroli, Jasmin, etc. occasionally used in confectionery for hard candies, syrups, etc.

It should be kept in mind that Ethyl anthranilate forms "Schiffs' bases" with most aldehydes and condensation products with many ketones. These reactions are accompanied by an increase in color and a noticeable change in odor/flavor.

G.R.A.S. F.E.M.A. No.2421.

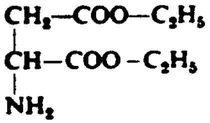
Prod.:

1) by direct esterification of Ethanol with Anthranilic acid preferably under azeotropic conditions.
2) from Isatoic acid and Ethanol by heating in a sealed tube.

4-14; 5-291; 26-540; 43-501; 44-1012; 86-16; B-XIV-319;

## 1155: ETHYL ASPARAGINATE

*d*-Diethyl aspartate.
Diethyl aminosuccinate.



$$\begin{array}{l} CH_2—COO—C_2H_5 \\ | \\ CH—COO—C_2H_5 \\ | \\ NH_2 \end{array}$$

$C_8H_{15}NO_4 = 189.22$

White crystals. M.P. 131° C. B.P. 227° C.

Soluble in water and alcohol, almost insoluble in oils.

In search of substitutes for salts and esters of aminoacids of flavor-enhancing effect, only a few chemicals have proved to be of any interest.

Usually, the esters have little effect on food products, partly because of their instability in aqueous acid media, and the Sodium salts are insoluble in alcohol or oils, therefore more or less eliminated from use in perfumery.

Various patents cover the use of Ethylesters of aminoacids as odor-enhancers in perfumery, but there is but little proof yet as to the value of the esters for that purpose.

Furthermore, Asparaginic acid is considered as "less important" in food, and it is classified as a non-essential amino acid.

The subject ester has – to the author's knowledge; only found experimental use so far.

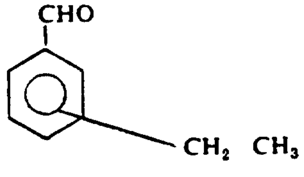
Prod.: by selective Ethylation of *L*-Aspartic acid. The acid can be obtained from the natural Asparagine, the *beta*-amide of the acid. It is found in Soybeans and other foods, and it can be produced synthetically.

1-293; 66-1108; 66-1109;

## 1156: ETHYL BENZALDEHYDE

Commercial products consists mainly of *para-* and *meta*-Ethyl benzaldehyde.

$C_9H_{10}O = 122.17$



Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Sweet, "Bitter-almond"-type odor, weaker, but more tenacious than that of Benzaldehyde. A slightly gassy, floral greenness is perhaps the most characteristic feature of the Ethylbenzaldehyde.

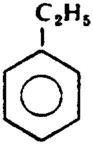
Suggested as a substitute for Benzaldehyde – which is rather unstable – in perfume compositions. It could find some use in mild florals, such as Lilac, Appleblossom, etc. and the aldehyde could also be used as a masking agent in industrial fragrances.

However, since very little Benzaldehyde is called for in perfumery, and since industrial fragrances demand very low-cost chemicals and oils, there has been very little interest in Ethylbenzaldehyde.

Prod.: from Ethyl toluene by oxidation. Ethyl toluene (mainly *para-*) is obtained by fractionation of gas oil.

## 1157: ETHYL BENZENE

Ethyl benzol.
Phenyl ethane.



$C_8H_{10} = 106.17$

Colorless mobile liquid. Sp.Gr. 0.87.
B.P. 136° C.

Insoluble in alcohol, miscible with oils and alcohol.

Sweet, but somewhat "gassy" odor. If at all reminiscent of any natural material, it would be a Hyacinth-type of gassy sweetness.

To the author's knowledge, this hydrocarbon is not used as such in perfumes or flavors, but it is a solvent for the extraction of certain natural materials, and could therefore occur as a trace impurity in those natural extracts.

Although it is flammable and its vapors form explosive mixtures with air (flash point 20° C.) it is considered much less dangerous than Benzene, and it is not considered toxic to human beings. Only very high concentrations present any health hazard to man. This is why Ethyl benzene is occasionally preferred over Benzene, and also because its much higher boiling point allows extraction temperatures well beyond 100° C. which may be necessary in certain rare cases.

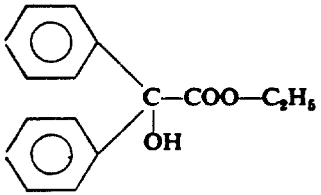
Prod.:

1) by Friedel-Crafts' reaction on Benzene, Ethylbromide and Aluminum chloride.
2) From Benzyl magnesium bromide and Diethyl sulfate.
3) From Ethylene plus Benzene plus Aluminum chloride.

26-540; 100-424; B-V-351; 68-107;

## 1158: ETHYL BENZILATE

Ethyl diphenylglycolate.



$C_{16}H_{16}O_3 = 256.30$

White or colorless crystals. M.P. 34° C.

This material is practically odorless, but imparts a bread-like flavor when incorporated in a flavor composition.

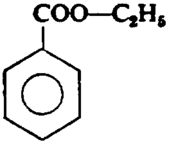
The ester was identified in bread more than 10 years ago (1955/56). It is interesting to note that Benzene derivatives are components of such common food as bread, when earlier it was generally believed that Benzol derivatives were rarely found in Nature (or in food).

Prod.: by esterification of Ethanol with Benzilic acid, e. g. under azeotropic conditions.

68-1134; 158-165; B-X-342;

## 1159: ETHYL BENZOATE

This ester is occasionally called "Niobe oil" commercially, but that name normally refers to the Methyl ester.



$C_9H_{10}O_2 = 150.18$

Colorless, slightly oily liquid. Almost insoluble in water, soluble in alcohol, miscible with most oils. Fairly soluble in Propylene glycol.

Sp.Gr. 1.04. B.P. 212° C.

Warm, floral-fruity, somewhat heavy odor, reminiscent of tropical flowers and with a faint resemblance to Methyl salicylate.

Sweet, somewhat heavy-fruity taste, remotely reminiscent of Black currant and Grape.

This ester is useful in perfume compositions of the more heavy-floral character, where Ylang Ylang is used, in Carnation, Tuberose and along with Labdanum in Leather fragrances, etc. It is quite powerful and the concentration in perfume compositions is normally limited to a few percent or less.

Finds extensive use in flavor compositions, ranging from imitation Banana, Blackcurrant and Cherry to Plum and Tobacco, Nut, Walnut and Liqueur. Also for Gooseberry, Cranberry, Strawberry, Currant, Vanilla and various fruit complexes.

The concentration in the finished product will normally be about 2 to 10 ppm, except in chewing gum where it may reach 60 ppm.

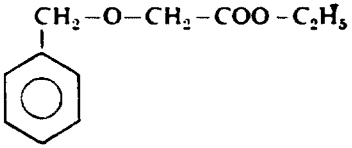
G.R.A.S. F.E.M.A. No.2422.
FCC-1964-819.

Prod.: By direct esterification of Ethanol with Benzoic acid under azeotropic conditions.

4-14; 5-256; 26-540; 43-501; 77-192; 86-16; 95-185; 96-205; 100-424; 106-147; 103-92; 155-80; B-IX-110; 140-149;

## 1160: ETHYL BENZOXYACETATE

Do not confuse with
Ethyl benzoyl acetate (see next monograph).



$C_{11}H_{14}O_3 = 194.23$

Colorless, slightly viscous liquid.
B.P. 248° C.

Sharp-floral, yet rather weak odor, remotely Jasmine-like, and of good tenacity.

Sharp, almost burning taste, not suitable for flavors.

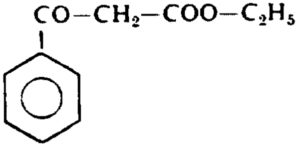
Has been suggested for use in perfume compositions, but does not seem to have any particular advantage over the conventional Jasmin chemicals. It does not even have the softness of Benzyl monochlororacetate, which is a comparatively pleasant odor, but uninteresting to the perfumer.

Prod.: by direct esterification of Ethanol with Benzoxyacetic acid.

31-159; 31-158;

## 1161: ETHYL BENZOYL ACETATE

Benzoyl acetic ester.



$C_{11}H_{12}O_3 = 192.22$

Colorless oily liquid. Sp.Gr. 1.12
B.P. 270° C. (decomposes).

Turns yellowish upon storage or when exposed to daylight.

Insoluble in water, soluble in alcohol, miscible with oils.

Peculiar Brandy-like odor of surprising tenacity (surprising mostly because one does not expect an aromatic-ethereal odor to be so lasting).

Slightly bitter taste, reminiscent of Whisky or fermented fruit.

This ester has, to the author's knowledge, no application in perfumes.

Finds some use in flavor compositions for imitation Whisky, and in various fruit complexes.

The concentration used corresponds to about 1 to 10 ppm in the finished product.

Prod.:

1) by condensation of Ethyl benzoate with Ethyl acetate in the presence of Sodium ethoxide (Claisen condensation type).
2) by condensation of Ethyl carbonate with Acetophenone. Catalyst is either Sodium ethoxide or Lithium amide.
3) As 1) – but using Ethyl acetoacetate in place of Ethyl acetate.

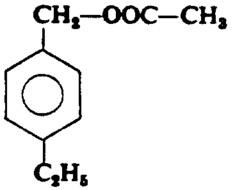
Ethyl benzoyl acetate can be hydrogenated and yield the interesting perfume material: Ethyl-*3*-hydroxy-*3*-phenylpropionate, which has a pleasant Labdanum character with the winey note of its parent keto-ester. (See that monograph).

G.R.A.S. F.E.M.A. No.2433.

26-426; 68-936; 77-192; 86-16; 100-424; B-X-674; 140-149;

## 1162: para-ETHYL BENZYL ACETATE

**Commercial products are mainly *para*-isomer, but they normally contain significant amounts of *ortho*- and *meta*-isomers.**



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-floral, slightly fruity odor of Jasmin-Gardenia type and good tenacity.

Has been suggested for use in perfume compositions and floral bases, mainly as a modifier for Benzyl acetate and "Tolyl acetate" (which is mainly *para*-Methyl benzyl acetate).

This material has greater tenacity than the conventional Jasmin esters, but it does not produce the powerful and radiant, sharp-floral note obtained with Benzyl acetate.

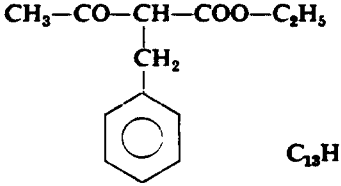
The trouble of having a commercial product with several isomers in variable proportion has also contributed to the failing success of subject material.

Prod.: by esterification of Ethylbenzyl alcohol (commercial prod. is *para*- with some *ortho*-isomer) with Acetic acid.

The alcohol can be obtained by selective catalytic reduction of Ethyl benzaldehyde.

## 1163: ETHYL BENZYL ACETOACETATE

Ethyl-*2*-acetyl-*3*-phenylpropionate.
Ethyl-*alpha*-acetyl hydrocinnamate.



$C_{13}H_{16}O_3 = 220.27$

Colorless liquid. Sp.Gr. 1.03. B.P. 280° C.

Insoluble in water, soluble in alcohol and oils.

Balsamic, fruity-floral odor reminiscent of Labdanum, with a distinct Jasmin-like note. There is an overall resemblance to the odor of Ethyl hydroxy phenylpropionate (see that monograph).

The flavor is sweet-herbaceous-fruity, somewhat "jam-like".

This material, although rarely found in the price lists of aromatic (perfume and flavor) chemicals, is frequently used in perfume compositions for Ambre creations, Jasmin bases, in Lavender or Citrus compositions etc.

It finds use in flavor compositions – always in mere traces – mainly in fruit flavors where it acts as a fixative and a "rounding-off" ingredient. Concentration may be about 0.1 up to 7 ppm in the finished product.

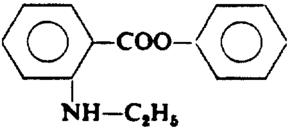
G.R.A.S. F.E.M.A. No.2416.

Prod.: from Benzyl acetoacetic acid and Ethanol, by esterification. Or by condensation of Ethyl acetate with Benzyl propionate.

4-14; 26-540; 155-80; B-X-710;

## 1164: N-ETHYL BENZYL ANTHRANILATE

Benzyl-*N*-ethylanthranilate.



$C_{15}H_{15}NO_2 = 241.29$

Pale straw-colored or almost colorless viscous liquid.

Insoluble in water, soluble in alcohol, miscible with oils, poorly soluble in Propylene glycol.

Rather heavy, fruity odor, remotely reminiscent of Raspberry (jam).

A rare chemical, this ester finds a little use in perfumes as a modifier in Orange blossom, Honeysuckle, Gardenia bases and in general as a fixative, sweet floralizer.

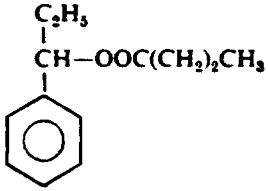
It has been suggested for use in flavor compositions as a fixative and as a background note in certain berry flavors, e. g. Raspberry, where a heavy-sweet undertone is occasionally desirable.

Prod.: by esterification of Benzyl alcohol with *N*-Ethyl anthranilic acid under azeotropic conditions, or with N-Ethylisatoic anhydride.

28-579;

## 1165: alpha-ETHYL BENZYL BUTYRATE

*alpha*-Phenyl propyl butyrate.
Ethyl phenyl carbinyl-*n*-butyrate.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid. Insoluble in water, soluble in alcohol, miscible with oils.

Powerful, fresh-fruity, sweet and slightly green odor.

Heavy-fruity, sweet, yet refreshing taste, not reminiscent of any particular fruit.

To the author's knowledge, this ester finds use in flavors only.

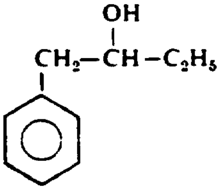
Mainly for fruity compositions, where it can introduce heavy, sweet undertones and tenacity. Concentrations are normally mere traces.

G.R.A.S. F.E.M.A. No.2424.

Prod.: by esterification of Ethyl phenyl carbinol with *n*-Butyric acid under azeotropic conditions.

## 1166: ETHYL BENZYL CARBINOL

Benzyl ethyl carbinol.
*alpha*-Ethyl-*beta*-phenylethyl alcohol.



$C_{10}H_{14}O = 150.22$

Colorless oily liquid, almost insoluble in water, soluble in alcohol and oils.

Sp.Gr. 0.98. B.P. 220° C.

Somewhat floral, earthy, wet-green, yet refreshing odor with some resemblance to Hyacinth, but not very powerful or tenacious.

Suggested for use in perfumery as a modifier in floral and herbaceous fragrance types, Hyacinth, New Mown Hay, Fougère, etc.

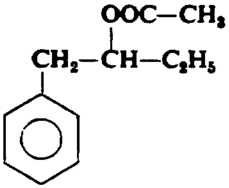
However, its lack of power and its limited field of application has made this chemical retire into oblivion, at least from the perfumer's point of view.

Prod.: (several methods) e. g. from Styrene oxide and Phenyl Magnesium bromide, a Grignard type reaction.

5-70; 31-23; 86-22; 103-289;

## 1167: ETHYL BENZYL CARBINYL ACETATE

Benzyl ethyl carbinyl acetate.
*alpha*-Ethyl-*beta*-phenylethyl acetate.



$C_{12}H_{16}O_2 = 198.14$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Fruity and slightly green, refreshing odor, not reminiscent of any particular fruit or natural product.

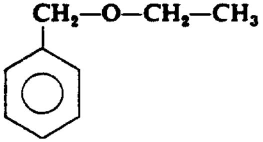
Has been suggested for use in perfume compositions, but it lacks the versatility of the conventional carbinols and esters, and it does not present any unusual odor characteristics.

The ester remains comparatively rare on the perfumery raw material shelf.

Prod.: by direct esterification of the carbinol.

## 1168: ETHYL BENZYL ETHER

Benzyl ethyl ether.



$C_9H_{12}O = 136.20$

Colorless, oily liquid. Sp.Gr. 0.95.
B.P. 187° C.

Insoluble in water, miscible with alcohol and oils.

Powerful, fruity, rather sharp odor, remotely reminiscent of Pineapple and Pear.

Somewhat sharp, fruity taste, rather nondescript.

This ether finds some use in flavor compositions, mainly in imitation Pineapple and in various fruit complexes.

Concentration is about 5 to 8 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2144.

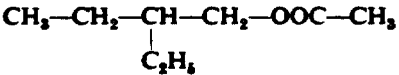
Prod.:
1) from Benzyl chloride and Sodium ethoxide.
2) from Benzyl alcohol by ethylation.

4-21; 68-502; 26-542; 86-22; 100-139;
B-VI-431;

## 1169: 2-ETHYL BUTYL ACETATE

*beta*-Ethyl butylacetate.
*3*-Methylolpentane acetate.
*2*-Ethyl-*1*-butanol acetate.
Pseudohexyl acetate.
Diethyl ethylacetate.

NOTE: The commercial literature on this item shows great confusion with respect to nomenclature.



$$CH_3-CH_2-\underset{\displaystyle C_2H_5}{\underset{|}{CH}}-CH_2-OOC-CH_3$$

$C_8H_{16}O_2 = 144.22$

Colorless liquid. Sp.Gr. 0.88. B.P. 163° C.

0.06% soluble in water, soluble in alcohol, miscible with oils.

Fruity, somewhat oily odor of rather nondescript type.

Sweet-fruity taste, reminiscent of Pear and Strawberry.

This ester is comparatively stable against hydrolysis, and finds therefore some use in soap perfumery to lend fruity notes and lift to the portion of the composition. It blends well with aldehydic and rosy fragrance types, and supports Geranium, Lavender or minty notes excellently.

Traces of the ester are occasionally used in flavor compositions for fruit complexes, etc. Usually about 5 to 8 ppm in the finished product.

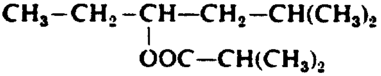
Prod.: by direct esterification of *3*-Methylol pentane.

G.R.A.S. F.E.M.A. No.2425.

4-15; (AB Bofors Nobelkrut data sheet).

## 1170: ETHYL-iso-BUTYLCARBINYL-iso-BUTYRATE

*2*-Methylhexan-*4*-yl-*iso*-butyrate.
*secondary*-*iso*-Heptyl-*iso*-butyrate.



$$CH_3-CH_2-\underset{\substack{|\\ OOC-CH(CH_3)_2}}{CH}-CH_2-CH(CH_3)_2$$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

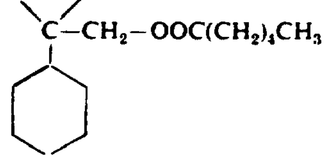
Oily-fruity, herbaceous odor of moderate tenacity. There is, again, an apparent lack of naturalness in the overall olfactory picture of this ester, and it seems to be characteristic of many of the related materials originating from large-volume industrial chemicals. One is tempted to blame the difficulty in describing such odors on the possible impurities in these materials, deriving from industrial intermediates, and only appearing on the perfumer's shelf because they are abundantly available, very inexpensive, and stable. But this is not always enough to compensate for an uninteresting odor.

The title material has found a little use in soap and detergent perfumes, and in masking compositions for industrial purposes.

Prod.: by direct esterification of Ethyl-*iso*-butylcarbinol with *iso*-Butyric acid. The carbinol is obtained from the corresponding ketone by hydrogenation. The ketone appears as a petrochemical and is produced in very large volume.

## 1171: ETHYL BUTYL CYCLOHEXYL CAPROATE

*3*-Methylolpentane cyclohexyl hexanoate.
Hexahydro diethyl phenylethyl caproate.



$C_{18}H_{34}O_2 = 282.47$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, but tenacious, oily-fruity, somewhat woody odor.

Fruity, but slightly bitter-dry taste.

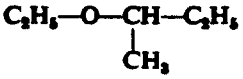
This ester was developed in a program of search for new fruity esters in the Pineapple family, and also as a natural result of extensive research in the Cyclohexane derivative field.

However, it has not shown any advantages over the existing and commercially available esters, and the author is of the impression that the subject material is practically obsolete.

Prod.: by esterification of *3*-Methylol pentane with Cyclohexane caproic acid.

NOTE: The literature shows considerable confusion with respect to nomenclature of this and related chemicals.

## 1172: ETHYL-secondary-BUTYLETHER



$C_2H_5—O—CH(CH_3)—C_2H_5$

$C_6H_{14}O = 102.18$

Colorless liquid. B.P. approximately 75° C.

Almost insoluble in water, soluble in alcohol, miscible with oils.

Extremely diffusive, fresh-fruity odor, somewhat fruity-oily.

This ether has been reported as interesting for the reconstitution of flavor in Orange juice.

Prod.: from Sodium ethoxide and *secondary*-Butyl chloride in the presence of a catalyst.

(Journal of Food Science, 29, (1964)).

## 1173: ETHYL-n-BUTYL KETONE

*3*-Heptanone.
Butyl ethyl ketone.

$C_2H_5—CO—(CH_2)_3CH_3$

$C_7H_{14}O = 114.19$

Colorless mobile liquid. B.P. 149° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Powerful, green-fatty, somewhat fruity odor.

Finds a little use in perfume compositions, but its diffusive power is difficult to control, as it requires considerable fixation to achieve a pleasant rate of evaporation.

The ketone is frequently used in flavor compositions, mainly in Melon types, Banana, and in certain types of Apple or fruit complexes.

Normal concentration is about 0.1 to 2 ppm in the consumer product, but it may occasionally be as high as 200 ppm in candy.

G.R.A.S. F.E.M.A. No.2545.

Prod.:
1) from *n*-Hept-*2*-yne by hydration.
2) by Grignard type reaction.
3) via Acetoacetic ester synthesis.

26-542; B-I-699;

## 1174: ETHYL-tertiary-BUTYL KETONE

*2,2*-Dimethyl pentan-*3*-one.
"Homo pinacone".
*2,2*-Dimethylpropione.

$C_2H_5—CO—C(CH_3)_3$

$C_7H_{14}O = 114.19$

Colorless liquid, almost insoluble in water, soluble in alcohol, miscible with oils.
Sp.Gr. 0.81. B.P. 125° C.

Camphoraceous-minty, rather harsh odor.

Bitter-camphoraceous taste.

Occasionally used in industrial fragrances as a masking agent.

Prod.: by treatment of Pinacone (Methyl-*tertiary*-butylketone) with Methyl iodide and Sodium amide. The process yields a number of homologues of subject material, and the Ethyl-*tertiary*-butyl ketone is the lowest boiling of these.

The ketone can also be produced from Pentamethyl ethylene glycol by dehydration and rearrangement.

31-91; 66-518; 66-506; 86-16;

## 1175: ETHYL BUTYL MALONATE

Butyl ethyl malonate.
Butylmalonic acid, diethylester.
"Butylmalonic ester".

$C_4H_9{-}CH(COO{-}C_2H_5)_2$

$C_{11}H_{20}O_4 = 216.28$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils. B.P. 236° C.

Mild, oily-fruity, somewhat ethereal odor of good tenacity.

Oily-fruity, but somewhat bitter taste unless highly diluted.

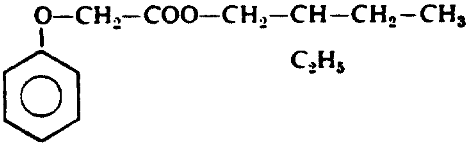
Finds use in flavor compositions, such as Apple and various fruit complexes. Concentration is normally limited to mere traces on account of the lack of sweetness in this ester.

Prod.: by condensation of Ethylvalerate with Ethyloxalate.

G.R.A.S. F.E.M.A. No.2195.

66-968;

## 1176: ETHYL BUTYL PHENOXYACETATE



$C_{14}H_{20}O_3 = 236.31$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Very mild, sweet-floral odor of excellent tenacity. When absolutely pure, the material often appears "odorless" to many observers. However, it does contribute interesting effects and nuances to certain types of fragrance, e.g. Rose, Jasmin, Magnolia, Peony, etc.

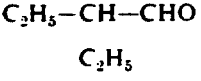
This ester is very rarely offered under its proper chemical name, but has been used in a number of perfume specialties and bases. Since it lends odor type and character obtainable with a large number of other materials, there has been relatively little demand for this ester.

Prod.: from *3*-Methylolpentane plus Phenoxyacetic acid.

4-14;

## 1177: 2-ETHYL BUTYRALDEHYDE

Pentane-*3*-carboxaldehyde.
Diethyl acetaldehyde.
*2*-Ethyl butanal.



$C_2H_5{-}\underset{C_2H_5}{CH}{-}CHO$

$C_6H_{12}O = 100.16$

Colorless mobile liquid. Sp.Gr. 0.82.
B.P. 118° C.

0.3% soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Powerful, oily-caramellic, "burnt" odor, reminiscent of notes from roasted Coffee and Cocoa beans.

Finds use in Chocolate imitation flavors.

The concentration of this aldehyde may be about 40 ppm in icecream, but is normally lower in other consumer products.

G.R.A.S. F.E.M.A. No.2426.

Prod.: from *1,1*-Diethyl ethylene oxide.

26-496; B-I-693;

## 1178: ETHYL BUTYRATE

Ethyl-*n*-butanoate.
Butyric ether*. (See footnote).
Commercial product is often: Ethyl-*iso*-butyrate (see next monograph).

$C_2H_5$—OOC—$(CH_2)_2CH_3$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 121° C.

0.5% soluble in water, miscible with alcohol and oils, soluble in Propylene glycol, almost insoluble in Glycerin.

Powerful, ethereal-fruity odor suggestive of Banana and Pineapple, and very diffusive.

Sweet, fruity taste, but not very powerful in aqueous media.

This ester has occasionally been used in minute traces in perfume compositions for its warm-fruity effect in Rose and other floral bases. It is also used as a masking agent for industrial fragrances. Its main use, however, is in flavor compositions for imitation Butter, Caramel, Cream, Cheese, Banana, Cherry, Grape, Orange, Peach, Rum, Walnut, and in Egg-nog flavor, various berry-compositions and fruit complexes (Tutti-frutti, etc.).

Concentration in baked goods may be about 30 to 100 ppm, while it can be up to 1400 ppm in chewing gum (Juicy-fruit-type).

G.R.A.S. F.E.M.A. No.2427.

Prod.: by esterification of Ethanol with *n*-Butyric acid under azeotropic conditions.

4-14; 26-542; 43-501; 43-732; 77-185; 86-16; 90-197; 107-211; 100-425; B-II-270; 103-90; 140-138;

* Butyric ether was – originally – the mixed Ethyl esters from the acids obtained from Butter by saponification. "Butter ether" was therefore not only Ethyl butyrate, but also Ethyl caproate, caprylate, caprate, etc. etc. Only 10% of the fatty acids in Butterfat are sufficiently low-molecular that they can produce esters of any significant flavor value. Butyric acid constitutes 3.5 to 4% of the total acids in Butterfat.

## 1179: ETHYL-iso-BUTYRATE

Ethyl-*iso*-butanoate.

$C_2H_5$—OOC—$CH(CH_3)_2$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.87.
B.P. 110° C.

Slightly soluble in water, soluble in alcohol and oils.

Diffusive, sweet-ethereal, fruity odor, milder and sweeter than that of the *n*-Butyrate. Overall more floral, less fruity than the *n*-Butyrate.

Sweet-fruity, not very powerful odor, not as pronounced Pineapple-Banana-like as that of the *n*-Butyrate.

Is occasionally used in soap perfumery where its greater stability makes it an interesting item for fruity topnotes. Ethyl-*iso*-butyrate is not as easily hydrolized as the *n*-Butyrate.

It is adviseable, however, to keep both esters absolutely dry in storage. The presence of even minute amounts of free acid is detrimental to the odor of the esters. For flavor use, it is not a serious drawback, since traces of free Butyric acids may even be desirable in fruity compositions.

This ester finds use in Butter, Cherry, Strawberry and various fruit complexes.

It is used in concentrations up to 200 ppm – e.g. in baked goods.

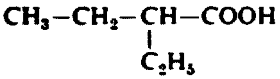
Prod.: by esterification of Ethanol with *iso*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2428.

4-16; 26-542; 43-732; 103-91; B-II-291;

## 1180: 2-ETHYL BUTYRIC ACID

Diethyl acetic acid.
*alpha*-Ethylbutyric acid.
Pentane-*3*-carboxylic acid.



$$\begin{array}{l} CH_3-CH_2-CH-COOH \\ \qquad\qquad\quad | \\ \qquad\qquad C_2H_5 \end{array}$$

$C_6H_{12}O_2 = 116.16$

Colorless liquid, slightly soluble in water, soluble in alcohol and oils. Sp.Gr. 0.92. B.P. 197° C.

Oily-fruity, acidulous odor, not as "rancid" as that of Caproic acid.

Fruity-earthy, acid taste with a Nut-like undertone.

The acid finds use in flavor compositions for imitation Nut and Walnut and in various fruit complexes.

The concentration will normally be about 35 ppm, e.g. in candy.

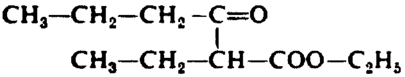
Prod.: by oxidation of *2*-Ethyl butyraldehyde.

G.R.A.S. F.E.M.A. No.2429.

26-496; 66-571; B-II-333;

## 1181: ETHYL BUTYRO BUTYRATE

Ethyl-*alpha*-butyryl butyrate.
The Ethyl butyryl-*iso*-butyrate is known, but is less interesting for the flavorist.



$$\begin{array}{l} CH_3-CH_2-CH_2-C{=}O \\ \qquad\qquad\qquad\qquad | \\ \qquad\quad CH_3-CH_2-CH-COO-C_2H_5 \end{array}$$

$C_{10}H_{18}O_3 = 186.25$

Colorless oily liquid. B.P. 211° C.

Peculiar deep-fruity, tart, "bitter-sweet" odor.

Fruity, tart, refreshing and quite powerful taste.

This ketoester is used in flavor compositions for imitation Blackcurrant, Blackberry, etc.

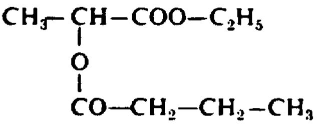
It is rarely offered commercially.

Prod.: from Ethyl butyrate by treatment with Sodium ethoxide.

4-15; 86-16; 86-17;

## 1182: ETHYL BUTYRYL LACTATE

Ethyl-*alpha*-butyryl lactate.
Lactic acid, ethyl ester, butyrate.



$$\begin{array}{l} CH_3-CH-COO-C_2H_5 \\ \qquad\;\, | \\ \qquad\;\, O \\ \qquad\;\, | \\ \qquad\;\, CO-CH_2-CH_2-CH_3 \end{array}$$

$C_8H_{16}O_4 = 188.23$

Colorless liquid.

Slightly soluble in water, soluble in alcohol and oils.

Fruity-buttery, sweet-sour odor of moderate to poor tenacity.

The taste in concentrations below 100 ppm is buttery, slightly fruity, but not conspicuously sour.

The title material is, to the author's knowledge, not used in perfumery.

It has found a little use in flavor compositions, mainly as a modifier in imitation Butter, Cream, Cheese, Milk, etc. and in various combination flavors, such as Butterscotch, Custard, etc.

Prod.: by acylation-esterification of Lactic acid.

The Butyl butyryl lactate (see monograph) is included in the American G.R.A.S. list, but the title material is not.

## 1183: ETHYL CAPROATE

Ethyl-*n*-hexanoate.
Ethyl hexoate.
Ethyl capronate.
Caproic ether.

$CH_3(CH_2)_4COO—C_2H_5$

$C_8H_{16}O_2 = 144.22$

Colorless liquid. Sp.Gr. 0.87. B.P. 165° C.

Insoluble in water, soluble in oils and alcohol. Poorly soluble in Propylene glycol, insoluble in Glycerin.

Powerful, diffusive, fruity-winey odor, suggestive of Apple, Banana, Pineapple, with a slightly floral undertone.

Traces of free Caproic acid will, naturally, greatly disturb the odor/flavor of this ester.

It finds some use in perfumery in the creation of modern fruity-floral topnotes, and it has often been used in connection with aliphatic aldehydes in mossy fragrance types, in which Allyl ionone may or may not be used at the same time. Minute traces can give interesting effects in Rose fragrances or bases, and it lends pleasant notes to Civet tincture, etc.

The ester is widely used in flavor compositions for imitation Apple, Pear, Banana, Cognac, Brandy, Grape, Pineapple, Strawberry, etc. Its comparatively powerful effect in flavors puts the limit of concentration to about 7 to 30 ppm calculated on the finished product, highest in chewing gum, lowest in soft drinks.

G.R.A.S. F.E.M.A. No.2439.
FCC-1964-821;

Prod.: by direct esterification of Ethanol with Caproic acid.

4-15; 26-542; 31-135; 43-501; 44-1230; 86-17; 100-425; 90-202; 103-91; B-II-323; 77-186; 140-141;

## 1184: ETHYL CAPROYL CAPROATE

Ethyl caproyl hexoate.

$CH_3(CH_2)_4CO—(CH_2)_5—COO—C_2H_5$

$C_{14}H_{26}O_3 = 242.36$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Sweet-winey-fruity odor of great tenacity.

Wine-like, Brandy-like taste with a pleasant herbaceous-fruity undertone.

This ketoester finds use in flavor compositions for imitation Brandy, Cognac, Wine, Cherry, Grape, Grapefruit, etc.

The use-concentration is normally limited to mere traces.

Prod.: from Ethyl caproate by treatment with Sodium ethoxide.

4-15; 86-17;

## 1185: ETHYL CAPRYLATE

Ethyl octylate.
Ethyl octanoate.
Ethyl octoate.

$CH_3(CH_2)_6COO—C_2H_5$

$C_{10}H_{20}O_2 = 172.27$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 209° C.

Insoluble in water and Glycerin, slightly soluble in Propylene glycol, soluble in alcohol, miscible with oils.

Fruity-winey, sweet odor, reminiscent of Apricot, Banana and Pineapple with a "fermented"-winey note.

Sweet-winey-brandy-like taste with a distinct fruity note.

The ester is only rarely used in perfumery.

It finds extensive use in flavor compositions for imitation Apricot, Apple, Brandy, Butter, Citrus fruits, Cheese, Grape, Nut, Pear, Pineapple, Rum, Strawberry, Banana, etc.

Concentration in the finished product is normally as low as 2 to 10 ppm, but it may amount to 60 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2449.

FCC-1964-823;

Prod.: by azeotropic esterification of Ethanol and *n*-Octanoic acid in presence of a catalyst.

4-15; 26-542; 31-124; 43-501; 86-17; 100-425; 103-91; B-II-348; 140-142;

## 1186: ETHYL CHLORACETATE

Ethyl monochloroacetate.
Chloroacetic ester.

$CH_2ClCOO—C_2H_5$

$C_4H_7ClO_2 = 122.56$

Colorless liquid. Sp.Gr. 1.16. B.P. 146° C.

Insoluble in water, miscible with alcohol and oils.

Ethereal, sweet odor. However, the vapors have eye-irritating effect which is sometimes ascribed to instantaneous hydrolysis of the ester in contact with mucous membranes.

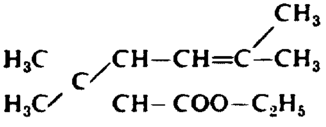
The ester has been suggested for use in flavor compositions, but the author believes that the use of it for such purpose is obsolete. Not only on account of uninteresting flavor (and odor) but also because of the hazard from possible traces of the corrosive Monochloroacetic acid.

Prod.: by hydrolysis of *1,2*-Dichlorovinyl ethyl ether. That material is produced commercially on a large scale.

26-542; 66-619; 100-426; B-II-197;

## 1187: ETHYL CHRYSANTHEMUMATE

Chrysanthemum-monocarboxylic acid, Ethyl-ester.
Chrysanthemic acid, Ethyl ester.
*1,1*-Dimethyl-*3*-(*beta-beta*-dimethylvinyl)-cyclopropanoic acid, ethyl ester.
*1,1*-Dimethyl-*3*-*iso*-butenyl cyclopropanoic acid(2)-ethyl ester.
Pyrethronic acid, ethyl ester.
*2,2*-Dimethyl-*3*-(*2*-methylpropenyl)-cyclopropane carboxylic acid, ethyl ester.



$C_{12}H_{20}O_2 = 196.29$

Colorless or very pale straw-colored oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, winey-herbaceous, sweet and ethereal, very pleasant odor of intriguing complexity, and with a powerfully lifting minty undertone. The spicy-herbaceous, warm and almost green-floral notes resemble certain notes in the Jasmin complex.

Overall, an odor that makes one think it would have to be a composition, not a single chemical.

It is quite possible that at least one of the commercially available products is a mixture of several isomers or homologues.

Although known only to few perfumers and flavorists, this ester has, in the author's opinion, very great possibilities in fragrances and in flavors. It is chemically related to Jasmone.

The winey character makes it an interesting topnote item for Citrus fragrances, and it lends a particularly pleasant effect to Bergamot. It enhances the effect of Clary Sage, and it rounds off the sharpness of aliphatic aldehydes. It blends excellently with the powerful natural floral materials, etc. Concentrations of much less than one percent may have quite satisfactory effect in perfume compositions.

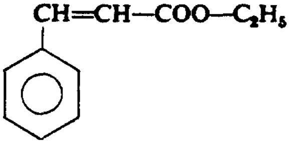
In flavors, it may enhance the effect of Cognac oil, or it can act as a fixative-blender in Pineapple, Banana, Brandy, Mango and many other types. Its greatest effects are probably in Rum and Pineapple.

The synthesis of the ester was completed only after World War II as the result of an intensive study of the active ingredients in Pyrethrum. The ester is now available at a very modest cost. It is also sold under various trade names.

67-99; 100-258;
Samples (among others): Benzol Products, Inc. (U.S.A.).

## 1188: ETHYL CINNAMATE

Ethyl-*beta*-phenylacrylate.
Ethyl-*3*-phenylpropenoate.
Ethyl-*trans*-cinnamate.



$C_{11}H_{12}O_2 = 176.22$

Colorless oily liquid, solidifying in the cold. M.P. 12° C. B.P. 271° C. Sp.Gr. 1.05.

Insoluble in water, soluble in alcohol, miscible with oils. Slightly soluble in Propylene glycol.

Sweet-balsamic, fruity-honey-like odor of excellent tenacity. Undertones of Orange (rather Orange-preserve-) or Grape-like character, and considerable overall power.

Sweet-fruity, Plum-Cherry-like taste of considerable power. This ester is used sparingly in perfume compositions ranging from Rose and fresh Ambre-like Citrus types to Chypres and Oriental fragrances. It imparts good fixation, and blends excellently with Styrax, Labdanum, Geranium, Citrus oils, Amyl salicylate, etc.

The ester is used widely in flavor compositions for imitation Cherry, Cinnamon, Grape, Peach, Plum, Raspberry, Spice, Strawberry, Vanilla, etc.

It performs particularly well in baked goods because of its stability and high boiling point. The concentration in finished products will normally be 4 to 40 ppm.

G.R.A.S. F.E.M.A. No.2430.

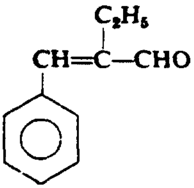
Prod.:

1) by direct esterification of Ethanol with Cinnamic acid under azeotropic conditions.
2) by Claisen-type condensation of Ethyl acetate and Benzaldehyde in presence of Sodium metal.

4-15; 5-267; 26-544; 43-501; 44-261; 44-461; 77-194; 86-17; 95-186; 100-426; 103-92; 106-148; 155-80; B-IX-581; 140-152;

## 1189: alpha-ETHYL CINNAMIC ALDEHYDE

*2*-Ethyl-*3*-phenyl-*2*-propenal-*1*.



$C_{11}H_{12}O = 160.22$

Pale yellowish, oily liquid. B.P. 256° C. Sp.Gr. 1.01.

Practically insoluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol.

Warm, oily-spicy, herbaceous odor, reminiscent of the condiment known as Capers, however, without the pungency or sharpness of that natural material. There is normally a Cinnamon-note in the aldehyde, but the author believes that it may vary according to the purity of the chemical. Overall a green-spicy odor, pleasant and with good tenacity.

In the long series of alkyl-substituted Cinnamic aldehydes, it seems that only the Amyl,-Hexyl- and Methyl-, perhaps to a minor degree the Butyl- have achieved any importance. The Ethyl- and the Propyl- are rarely found on the perfumer's shelf, or even in the research files.

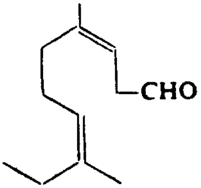
This aldehyde could find some use as a modifier in modern herbaceous and herbaceous-floral or spicy compositions, but it would have to be commonly available before any perfumer would consider using it regularly. It does not offer any very unusual tonalities and may therefore never become a standard item in perfumery.

Prod.: by condensation of Benzaldehyde with Butanal (*n*-Butyl aldehyde) in hydro-alcoholic dilution and usually in the presence of a catalyst.

31-51;
see also: Aetherische Oele, Riechstoffe, Parfumerien, Essenzen und Aromen, July 1953, page 148.

## 1190: ETHYL CITRAL

*3*,*7*-Dimethyl-*2*,*6*-nonadien-*1*-al.
"Homocitral".
The name "Ethyl citral" is therefore a misnomer, but commercially used and accepted in the same way as e.g. "Ethyl vanillin" etc.



$C_{11}H_{18}O = 166.27$

Almost colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils. Somewhat soluble in Propylene glycol.

Powerful and diffusive, fresh lemony odor, richer than that of Citral, but less sharp. The "Ethyl citral" also lacks the peculiar (and mostly undesirable) caramellic note of commercial synthetic Citral, and it is longer lasting. This type of odor is sometimes referred to as an "Epoxy-odor".

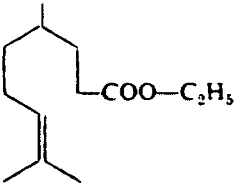
This higher homologue of Citral is suggested for use in perfume compositions as a modifier for Citral, a substitute with greater tenacity and a "new" lemony odor.

The cost of this aldehyde is, however, somewhat prohibitive, and presents a hard competition from the much less expensive Citral.

This aldehyde can be produced from Ethyl geraniol.

Sample and data: Hoffmann-la Roche Aromatics, Inc. (U.S.A.).

## 1191: ETHYL CITRONELLATE



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

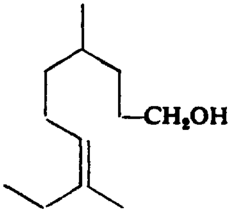
Fresh, green (foliage-type) rosy odor, not very tenacious. Overall resembling the fresher, initial notes in Geranium. This ester is very rarely offered commercially and has, in the author's opinion, little more than academic interest. It is too expensive for what it has to offer, but it may occasionally find its way into various artificial essential oils.

Prod.: by esterification of Ethanol with Citronellic acid.

28-607; 90-240; 90-241; 4-15;

## 1192: ETHYLCITRONELLOL

"Homocitronellol".
*3*,*7*-Dimethyl-*6*-nonen-*1*-ol.
Commercial product contains a considerable amount of Ethyl geraniol.



$C_{11}H_{22}O$ = 170.30

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Mild-rosy, but not distinctly floral odor, weaker than that of Citronellol, more oily-waxy and fruity.

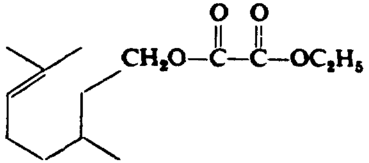
In view of the character and lack of power of this item, there is little chance that it will ever become an important perfume material.

It is very rarely offered commercially.

7-124; 86-17;

## 1193: ETHYL CITRONELLYL OXALATE

Citronellyl ethoxalate.
Citronellyl ethyloxalate.
Presumably a component of "Malvone" and "Ambrettozon".



$C_{14}H_{24}O_4$ = 256.35

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

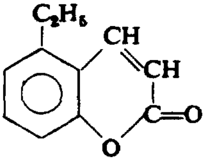
Sweet, floral-musky odor with notes resembling those of Labdanum and Ambrette seed, or the sweet notes of Ambregris.

The chemical as such is rarely offered commercially, but it is incorporated in many specialties, mainly those intended for fixation of floral and Ambre-like notes, etc.

28-587;

## 1194: 5-ETHYL COUMARIN

"Cumaran".



$C_{11}H_{10}O_2$ = 174.20

White or colorless crystals. M.P. 70° C.
B.P. 300° C.

Very slightly soluble in cold water, somewhat soluble in boiling water, fairly soluble in alcohol, soluble in oils. Almost insoluble in Propylene glycol.

Heavy-sweet, herbaceous and nut-like odor with an oily-balsamic undertone. Overall with some resemblance to the lower Cinnamates.

Although rarely offered commercially, this lactone finds some use in perfume compositions of the floral type, or in support of Honey-like notes or background sweetness in Oriental fragrances, etc.

This material remains, however, rather expensive, and it is doubtful whether it can become a standard item on the perfumer's shelf.

Prod.: e.g. from Salicylic aldehyde plus Butyric anhydride and Sodium butyrate (Perkin's synthesis).

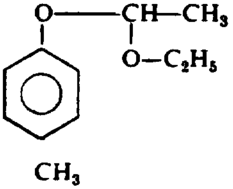
96-180; 37-726; 86-17; 4-36; 103-303;

6-ETHYL COUMARIN has been mentioned in the perfumery literature (28-255) but the author believes that this isomer is of no importance to the perfumer. It is apparently not commercially available.

## 1195: ETHYL-para-CRESYL ACETAL

Acetaldehyde ethyl-*para*-cresylacetal (a mixed Acetal).

This material has at times been called:
Methyl-*para*-cresyl acetal, sometimes confused with the Ethyl-acetal.



$C_{11}H_{16}O_2 = 180.25$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Warm, spicy-floral, herbaceous odor of considerable tenacity. Various samples have shown either anisic sweetness or cresylic harshness, while material, believed to be olfactorily pure has a distinctly floral, although rather heavy odor.

This acetal has been used in perfume compositions for heavy floral bases, Tuberose, Jasmin, Orangeblossom, etc. and as a modifier for spicy-floral materials, sweet-balsamic odors, etc.

It is rarely offered under its proper chemical name, but it forms part of certain perfumery specialties.

Prod.: from *para*-Cresol plus Ethyl-*alpha*-chloroethylether and Methyl vinylether.

## 1196: ETHYL CROTONATE

Ethyl-2-butenoate.
Ethyl-*alpha*-crotonate.

$CH_3—CH{=}CH—COO—C_2H_5$

$C_6H_{10}O_2 = 114.15$

Colorless mobile liquid. Sp.Gr. 0.92.
B.P. 136° C.

Almost insoluble in water, soluble in alcohol and oils.

A solid modification, which is generally considered more stable, consists of white needle-like crystals, M.P. 42° C. – very slightly soluble in water, soluble in alcohol and oils. B.P. 200° C.

The commercial Ethyl crotonate, used in flavor compositions, is a liquid.

It has a powerful and diffusive, sour-caramellic-fruity odor, reminiscent of unripe berries.

This ester is used in imitation Strawberry, occasionally also in Pineapple or other imitation fruit flavors.

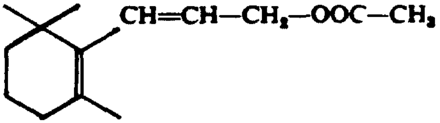
The concentration used is generally very low, classified as "traces" only.

Prod.: by esterification of Ethanol with Crotonic acid under azeotropic conditions.

26-544; 66-633; 90-220; B-II-440;

## 1197: ETHYL CYCLOCITRYLIDENE ACETATE

"Resedone".



$C_{14}H_{22}O_2 = 222.33$

Colorless oily liquid.

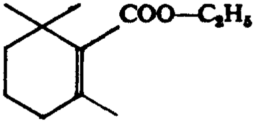
The odor of this rare chemical is described as green, earthy, oily, resembling Violet and Reseda. It is quite possible that this material appears as chief component in one or two well-known specialties, sold under trade names.

Yet, there seems to have been very little interest in perfume materials of this odor type, and it may become obsolete within the next decade or so.

Prod.: from Cyclocitrylidene ethanol by Acetylation.

31-125; 4-38;
see also: Methyl cyclocitrylidene acetate.

## 1198: ETHYL-beta-CYCLO GERANIATE



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.

Refreshing, oily-green, vegetable or Apple-like odor.

This material has been suggested for use in perfume compositions as a modifier for Geranyl and Citronellyl esters and in Geranium bases, etc.

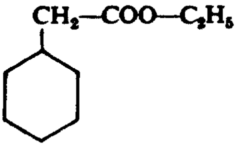
The chemical is very rarely offered commercially, and it is not likely that it will become very popular on the perfumer's shelf. It does not offer any unique or outstandingly new notes.

Prod.: from *beta*-Cyclogeranic acid and Ethanol.

28-579;

## 1199: ETHYL CYCLOHEXANE ACETATE

Cyclohexaneacetic acid, Ethylester.
Ethyl hexahydrophenylacetate.
NOTE: Nomenclature – see footnote under this monograph.



$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful fruity odor of Raspberry-Apple type, but in no way a "natural" fruit odor. Moderate tenacity.

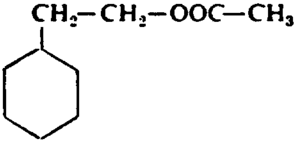
Powerful sweet-fruity taste at concentrations below 10 ppm, and with useful effects well below that mark.

This ester is used in flavor compositions in Europe and other countries, but it is not approved for food flavors in the U.S.A. It is possible that confusion with very closely related chemicals contribute to the apparent lack of interest in this ester. Until it is generally and officially approved for food flavor use, the material could find good use in perfume compositions, where its power and sweet fruity notes blend well with Jasmin fragrances for detergents and household products. It performs particularly well in hot water partly because of its insolubility in water, bringing the fragrance out and, for example, largely outperforming Benzylacetate in this respect.

This particular ester is quite popular in European flavor creation, and it is most conceivable that it eventually will be approved in the United States og America.

Prod.: by direct esterification of Ethanol with Cyclohexane acetic acid, preferably using azeotropic conditions.

NOTE: A very common confusion is that with Hexahydro phenylethylacetate:



$CH_2-CH_2-OOC-CH_3$

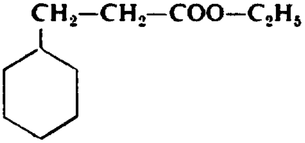
See that monograph under the title:
Ethyl cyclohexyl acetate, the name with which the subject ester is most freqently confused.

The author has preferred to use the common perfumery literature names as head names, and indicate the correct chemical names as synonyms.

140-144;

## 1200: ETHYL CYCLOHEXANE PROPIONATE

Cyclohexanepropionic acid, Ethylester.
Ethyl hexahydrophenylpropionate.
See note below about nomenclature.



$CH_2-CH_2-COO-C_2H_5$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity odor of Pear-Peach-Banana type, but only in extreme dilution displaying a natural fruit odor.

Sweet and fruity taste in dilutions of about 10 ppm. The power is considerably greater than that of the conventional alifatic esters.

This ester is used in Europe and other countries in flavor compositions for candy, etc. In fact, the esters of Cyclohexane acetic acid, Cyclohexane propionic acid and a few homologues, are quite popular outside of the United States of America. They are usually applied in conjunction with the lower alifatic esters to increase the overall power of the flavor.

Prod.: by direct esterification of Ethanol with Cyclohexane propionic acid under azeotropic conditions.

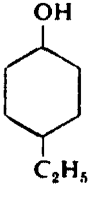
140-144;

NOTE: The Propionic ester of Cyclohexylethanol is known, and it finds limited use in perfumery and flavors.

It is mentioned in this work under the head name:
Ethyl cyclohexyl propionate, and there are many cases of confusion between the two esters. See also Ethyl cyclohexane acetate.

## 1201: para-ETHYL CYCLOHEXANOL

*1*-Hydroxy-*4*-ethyl cyclohexane.
Do not confuse with: Cyclohexyl ethanol, which is Hexahydro phenylethyl alcohol.



$C_8H_{16}O = 128.12$

Colorless oily liquid.

Sweet, but rather pungent, gassy odor with a floral undertone.

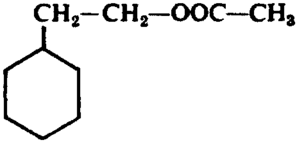
In the author's opinion, this material is not used as such in perfumery, except perhaps in certain types of masking odors for industrial purposes. But it serves as an intermediate in making more interesting perfume chemicals. It was used in the early 1930's as a modifier in Hyacinth and other floral fragrance types.

Prod.: by catalytic hydrogenation of *para*-Ethyl phenol.

86-17;

## 1202: ETHYL CYCLOHEXYL ACETATE

Cyclohexane ethylacetate.
Hexahydro phenylethyl acetate.



$C_{10}H_{18}O_2 = 170.25$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity odor of considerable tenacity. The fruitiness is of rather nondescript character, which is almost typical of the Ethyl- and Methyl-cyclohexanol esters, but their sweetness and power exceed that of the corresponding Benzyl- or Phenylethyl esters.

Sweet and distinctly fruity taste in high dilution, reminiscent of Raspberry. This ester is used in fruit and Honey imitation flavors at concentrations equivalent to about 20 ppm in the finished product. It acts partly as a blender, partly as a fixative for some of the more volatile alifatic fruit esters, or the lower Phenylacetates in Honey bases.

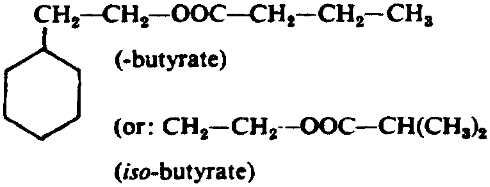
G.R.A.S. F.E.M.A. No.2348.

Prod.: by esterification of Cyclohexyl ethanol with Acetic acid or Acetic anhydride.

86-17;

## 1203: ETHYL CYCLOHEXYL BUTYRATE

Cyclohexane ethylbutyrate.
Hexahydro phenylethyl-*n*-butyrate.
NOTE: The *iso*-butylester of Cyclohexylethanol is also a commercially available item, offered for perfumery use. The author believes that the name "-butyrate" is commonly used for the *iso*-butyrate.



$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Powerful, sweet, deep-fruity, almost "jam-like" odor. Not reminiscent of any particular fruit, perhaps remotely Apricot-Plum-like.

Sweet, fruity, "marmelade"-like taste in high dilution.

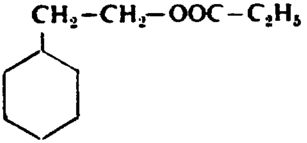
This ester has been suggested for use in various fruit complexes and other flavor bases.

It is not listed in the American G.R.A.S. list, and may temporarily be confined to use in fragrances, where a heavy fruity note may be desirable, e.g. in combination with Undecanolide or Ethyl Methyl Phenyl glycidate, etc. for lipstick fragrances, hand creams, hair sprays, etc. and in various masking problems.

Prod.: from Cyclohexyl ethanol by esterification with *iso*-Butyric acid under azeotropic conditions.

## 1204: ETHYL CYCLOHEXYL PROPIONATE

Cyclohexane ethyl propionate.
Hexahydro phenylethyl propionate.



$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid, insoluble in water, soluble in alcohol and oils.

Powerful, fresh-fruity, sweet odor with some resemblance to that of Pineapple.

Sweet, fresh-fruity, Pineapple-like taste in high dilution.

This ester is suggested for use in perfumery, mainly in fragrances for household products, where power and low cost partly monitors the creation. It finds some use in flavor compositions, mainly as a power factor in Pineapple imitations, and as a modifier for the conventional Allylcaproate and Allyl cyclohexane propionate. It is sweeter than both, but less typical of Pineapple.

The concentration used is normally about 30 ppm in candy.

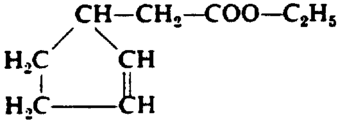
G.R.A.S. F.E.M.A. No.2431.

Prod.: by esterification of Ethyl cyclohexanol with Propionic acid or Propionic anhydride.

See also Ethyl cyclohexane propionate.

## 1205: ETHYL CYCLOPENTENYL ACETATE

Cyclopentenyl ethyl acetate.
NOTE: The author believes that the material called: Ethyl cyclopentenoate in commercial literature is actually Ethyl cyclopentenyl acetate.
Cyclopent-*2*-ene acetic acid, Ethylester.



$C_9H_{14}O_2 = 154.21$

Colorless mobile liquid.

Powerful, fresh-fruity odor with notes of "overripe" Pineapple, a remote resemblance to Ethyl valerate, but far more powerful and diffusive, greener and sharper.

This ester finds some use in flavor compositions as a trace component in imitation Apple, Rum, Pineapple, Strawberry, Melon, etc. and minute traces can also be useful in certain types of Lemon and Lime, to introduce the green freshness of the rind.

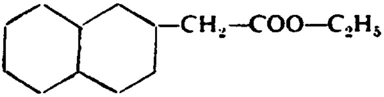
The ester has little, if any, application in perfumery.

Prod.: by esterification of Ethanol with Cyclopentene acetic acid.

86-39; 4-15;
see also: Methyl cyclopentenyl acetate.

## 1206: ETHYL DECAHYDRO-beta-NAPHTHYLACETATE

Decahydro-*beta*-naphthylacetic acid, ethyl ester.



$C_{14}H_{24}O_2 = 224.35$

Colorless viscous liquid. B.P. 246° C.

Insoluble in water, soluble in alcohol, miscible with perfume oils.

Faint, but tenacious, mild-fruity, "canned-fruit"-like odor, reminiscent of Quince and Pear.

The flavor is remotely reminiscent of Quince or Melon.

Has been suggested for use in perfumes and flavors for its peculiar, delicately fruity note.

The ester is very rarely offered commercially and has not achieved any significant degree of popularity.

Prod.: from Decahydronaphthylacetic acid and Ethanol, by esterification.

31-127;

## 1207: ETHYL DECIN CARBONATE

Ethyl dec-*l*-yne-*l*-carboxylate.
Ethyl undecynoate.
"Mignonette".
Commercial products (under trade names in particular) are often mixtures of Methyl- and Ethyl decin carbonates.

$CH_3(CH_2)_7{-}C{\equiv}C{-}COO{-}C_2H_5$

$C_{13}H_{22}O_2 = 210.32$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Green and slightly earthy, herbaceous-rootlike odor, reminiscent of Reseda. Considerably softer than the Heptin- and Octin carbonates. Comparatively tenacious.

This rare ester is occasionally used in perfumery for topnote effects in various floral fragrance types, in many herbaceous types, and in certain Citrus types. The use of acetylenic esters has decreased significantly since the appearance of commercially available Hexenyl esters and homologues, all of which produce more natural-green notes in great variation. The use of Reseda type fragrances is extremely rare now.

Prod.: (several methods) e.g. from Nonyl aldehyde, or from Decyne, via Decyne sodium to the acetylenic acid and finally esterification.

31-124; 4-15;

## 1208: ETHYL DECYLATE

Ethyl caprate.
Ethyl caprinate.
Ethyl decanoate.

$CH_3(CH_2)_8COO{-}C_2H_5$

$C_{12}H_{24}O_2 = 200.32$

Colorless oily liquid. Sp.Gr. 0.86. B.P. 245° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Sweet, oily-nutlike odor with a rich, wine-yeast type background. Oily, "Brandy-residue"-like flavor.

This ester finds a little use in perfumery, mainly for certain types of floral bases, where a fatty-waxy note is desirable in the creation of "petal"-like effects, e.g. Tuberose, Lily, Narcisse, Rose, etc. Although Tulips are generally considered odorless, this ester is probably one chemical that can recall the odor of the common Gardentulip flower best, out of all single chemicals.

The subject material is widely used in flavor compositions, for imitation Arak, Rum, Brandy, Whisky, Cognac, and in Peach, Strawberry, Grape (white and green Grapes), Cherry, Pineapple, Plum, etc. as well as in various types of Liqueur flavors.

Concentration in the finished product will normally be about 2 to 25 ppm.

G.R.A.S. F.E.M.A. No.2432.

Prod.: by direct esterification of Ethanol with Decanoic acid under azeotropic conditions.

4-15; 26-542; 77-187; 86-17; 90-213; 103-91; B-II-356; 140-143;

## 1209: ETHYL DECYL ETHER

Decyl ethyl ether.

$CH_3(CH_2)_9—O—C_2H_5$

$C_{12}H_{26}O = 186.34$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Fatty-oily, yet refreshing and "clean" odor of moderate tenacity.

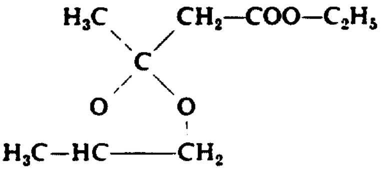
This ether has been suggested for use in perfume compositions, e.g. for detergent perfumes, soap perfumes, etc., where at times a "fresh-laundry" type of odor is desirable. In such cases, the subject ether may serve as a modifier for Dodecanal and Dodecanol etc.

This material is rarely offered commercially.

Prod.: e.g. by reacting Sodium ethoxide with Decyl bromide in Ethyl alcoholic solution.

## 1210: ETHYL-2,4-DIMETHYL-1,3-DIOXOLANE-2-ACETATE

Fructone B (I.F.F.).



$C_9H_{16}O_4 = 188.23$

Colorless or pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol, miscible with oils.

Fruity-floral and warm, sweet odor of good tenacity. The winey-"fermented-fruit-like" undertones resemble the odor of Strawberry preserve ("cooked Strawberry odor").

This ketal type of chemical has found some use in perfume compositions where a certain deep-fruity note is desirable along with a floral complex. Jasmin, Tuberose, Gardenia and many other floral bases, spicy fragrances, etc. can achieve new and interesting "lifts" from this material, which has an overall effect resembling that of the alkyl-substituted Cyclopentenones and their homologues.

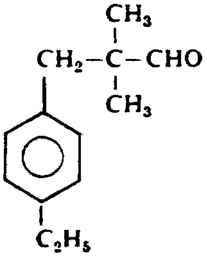
Prod.: from Propylene glycol and Ethyl acetoacetate. The latter acts as a ketone to condense with the glycol. The condensation is normally encouraged by a catalyst and carried out under conditions of azeotropic distillation.

See also: Ethyl-*2*-methyl-*1,3*-dioxolane-*2*-acetate.

## 1211: para-ETHYL-alpha-alpha-DIMETHYL HYDROCINNAMIC ALDEHYDE

*para*-Ethyl-*alpha*-*alpha*-dimethyl phenylpropyl aldehyde.

*2,2*-Dimethyl-*3*-(*para*-Ethylphenyl)-propanal-*1*



$C_{13}H_{18}O = 190.29$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Fresh, floral-green, cool and vegetable-juicy odor, remotely reminiscent of Cucumber and Cyclamen. Comparatively powerful and tenacious.

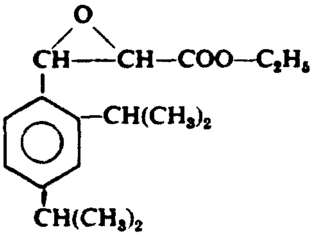
Has been suggested for use in perfume compositions as a modifier for Cyclamen aldehyde. It is somewhat greener and less nauseating-sweet, but it does not have the versatility of Cyclamal.

This aldehyde is very rarely offered under its proper chemical name.

Prod.: many methods, mostly using *para*-Ethyl benzaldehyde as a starting material, other methods from *para*-Ethyl benzylchloride.

## 1212: ETHYL-2,4-DI-iso-PROPYL PHENYLGLYCIDATE

Ethyl-*alpha-beta*-epoxy-*beta*-(-*2,4*-di-*iso*-propylphenyl)-propionate.



$C_{17}H_{24}O_3 = 276.38$

Colorless or pale straw-colored, viscous liquid. B.P. 315° C.

Insoluble in water, soluble in alcohol and oils.

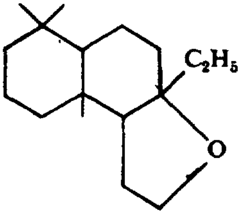
Faint, but very tenacious and pleasant, sweet-Ambre type odor, so discrete, that many observers find it rather musky, a description often applied to chemicals of very faint, but persistent odor. There is a possibility of confusion, and one of contamination in the fact that the aldehyde corresponding to this glycidate has an odor resembling that of Musk.

The subject aldehyde is very rarely offered commercially, and it does not seem to present any substantial advantages over the more modern Musk and Ambregris materials, many of which can be manufactured at lower cost.

Prod.: by condensation of *2,4*-Di-*iso*-propylbenzaldehyde with Ethyl monochloro acetate.

5-326; 17-34; 86-17;

## 1213: 3a-ETHYL-DODECAHYDRO-6,6,9a-TRIMETHYLNAPHTO-(2,1-b)-FURAN



$C_{17}H_{30}O = 250.43$

Colorless, viscous liquid.

Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

This bicyclic oxide, which is the next higher homologue after the well-known specialty "Fixateur 404" of Firmenich Co., has been suggested for use in perfume compositions.

It has a very tenacious, dry-woody Ambregris-type odor of delicate effect and yet of great power. Its high cost is partly compensated for by the fact that it may be used at concentrations below one percent in the perfume oil or base with perceptible effect.

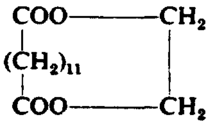
Usually marketed under trade name, this chemical has a place in creative perfumery, although it has strong competition from lower-cost, long-time available similar chemicals.

Prod.: (several methods) from Manool or Sclareol, both natural isolates, or purely synthetic.

See also: Dodecahydro-*3a,6,6,9a*-tetramethyl-(*2,1-b*)-furan, and: Fixateur 404.

## 1214: ETHYLENE BRASSYLATE

Ethylene tridecane dioate.
Ethylene undecane dicarboxylate.
Cyclic ethyleneglycol ester of brassylic acid.
"Musk T" (Takasago Perfumery Co., Ltd.).
Astrotone (Usine Chimiques Rhone-Poulenc).
Tridecane dioic acid, cyclic Ethyleneglycol diester.
Cyclo-*1,13*-ethylenedioxytridecan-*1,13*-dione.
- and many other trade names.



$$\begin{array}{ll} COO & \text{—} CH_2 \\ (CH_2)_{11} & \quad | \\ COO & \text{—} CH_2 \end{array}$$

$C_{15}H_{26}O_4 = 270.37$

Almost colorless, viscous liquid. Solidifies in the cold, melts at about minus 5° C. B.P. approximately 332° C. Sp.Gr. 1.05.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Sweet-musky, somewhat oily odor of outstanding tenacity.

This cyclic ester was introduced into perfumery only a few decades ago, and has grown to become one of the most important musk chemicals to the perfumer. After many years as a captive chemical and at a very high cost, it has reached almost every perfumer's shelf and is available at less than one-sixth of the original cost.

It is used extensively in perfumery as a fixative and intensifier of sweet-floral notes. One very well-known fragrance type contains an unusually large proportion of this ester with Undecanolide as one of its companions. This combination results in quite unusual lasting qualities of that perfume type. So much that some people dislike it just for that reason.

Ethylene brassylate has a perceptible effect usually at concentrations starting below one percent in the perfume base or oil. Normal use-concentration is about 0.5 to 3.0 percent. It is stable in soap and does not cause discoloration. Poorer grades of this ester tend to develop fatty-rancid, almost Castor-oil-like off odors upon ageing.

The use of this material in flavor compositions as a fixative and "rounding-off" agent has been suggested.

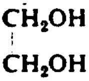
It finds use as an ageing or "maturing"-agent in alcohol for perfume solution purposes.

Prod.: from Ethylene glycol and Brassylic acid.

4-13; 86-15; 86-17; 31-129; 156-251; 156-267; 157-82;

## 1215: ETHYLENE GLYCOL

*1,2*-Ethanediol.
Glycol.



$$\begin{array}{l} CH_2OH \\ | \\ CH_2OH \end{array}$$

$C_2H_6O_2 = 62.07$

Colorless, somewhat viscous liquid, miscible with water and alcohol, soluble in lower alifatic alcohols and ketones, Propylene glycol and Glycerin, poorly soluble in Hydrocarbons such as Terpenes as well as in Terpene alcohols, esters, etc. Sp.Gr. 1.12. B.P. 198° C. Hygroscopic.

Faint, musty odor. Warm and sweet taste in water.

This material serves as a solvent in perfumery, but has mostly been replaced by more versatile solvents such as Triethylene glycol, Dipropylene glycol, Hexylene glycol, etc. all of which are superior solvents for most perfume materials.

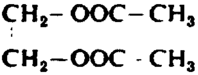
Ethylene glycol has been used as a diluent for flavor compositions but the use of this glycol in food products has been abandoned in most countries now. Ethylene glycol is considered moderately toxic, but the reports on minimum lethal dosis for human beings vary enormously. It is generally believed that a few grams may kill an adult person.

Prod.: from Ethylene oxide by hydration.

26-564; 100-429; B-I-465; 77-173; 140-128;

## 1216: ETHYLENE GLYCOL DIACETATE

Glycol diacetate.
Ethylene acetate.



$$\begin{array}{l} CH_2-OOC-CH_3 \\ | \\ CH_2-OOC-CH_3 \end{array}$$

$C_6H_{10}O_4 = 146.15$

Colorless liquid. Sp.Gr. 1.12. B.P. 190° C.

14% soluble in water, miscible with alcohol and oils. Poorly soluble in Propylene glycol.

Faint, sweet, oily-winey odor.

Slightly bitter taste at concentrations of 50 ppm or higher in water.

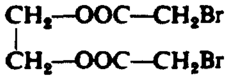
Has been suggested for use in flavor work, mainly as a solvent or co-solvent, e.g. when compositions of Citrus oils call for special solvents or in other cases where Propylene glycol is an unsufficient solvent.

This material has no value as a perfume or flavor material.

Prod.: by direct esterification of Ethylene glycol with Acetic acid, using azeotropic conditions.

160-1018;

## 1217: ETHYLENE GLYCOL DI-MONOBROMACETATE



$$\begin{array}{l} CH_2{-}OOC{-}CH_2Br \\ | \\ CH_2{-}OOC{-}CH_2Br \end{array}$$

$C_6H_8Br_2O_4 = 303.96$

Colorless oily liquid. Sp.Gr. 1.80.

Very slightly soluble in water. Miscible with alcohol. Soluble in Ethylene glycol.

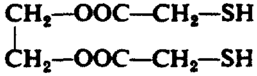
Faint, ethereal odor (when pure).

This peculiar ester has served as a powerful fungicide or fungistat in carbonated beverages, beer, Orangeades, and many other aqueous beverages or food products.

The use of this ester is prohibited in many countries. Effective concentrations vary according to the Nature of the functional product, but may be about 2 to 20 ppm. The ester hydrolyzes slowly in aqueous products and the toxicity hazard decreases simultaneously.

Prod.: by esterification of Ethylene glycol with Monobromacetic acid under azeotropic conditions.

## 1218: ETHYLENE GLYCOL-DITHIOGLYCOLATE



$$\begin{array}{l} CH_2{-}OOC{-}CH_2{-}SH \\ | \\ CH_2{-}OOC{-}CH_2{-}SH \end{array}$$

$C_6H_{10}O_4S_2 = 210.28$

Colorless liquid, poorly soluble in water, miscible with alcohol. Sp.Gr. 1.31.

The odor varies according to origin and to the quality of the Thioglycolic acid used in the manufacture of the ester. Poorer grades yield esters of Hydrogen-sulfide-type odor.

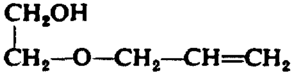
This ester has little more than academic interest, but it may be formed in small quantities in cosmetic preparations when Thioglycolic acid and Ethylene glycol are used at the same time.

Prod.: by esterification of Ethylene glycol with Thioglycolic acid.

34-1245;

## 1219: ETHYLENE GLYCOL MONOALLYL ETHER

Allyl cellosolve.
Allyl glycol (mono-).



$$\begin{array}{l} CH_2OH \\ | \\ CH_2{-}O{-}CH_2{-}CH{=}CH_2 \end{array}$$

$C_5H_{10}O_2 = 102.14$

Colorless liquid. Poorly soluble in water, soluble in alcohol and oils.

Peculiar, earthy, mushroom-like odor.

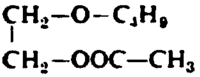
The odor of this ether is too weak and too rarely wanted that this material can become popular. It will probably remain a rare item on the research shelf.

The flavor is rather uninteresting, and does not resemble that of mushroom.

Prod.: from Allyl alcohol and Ethylene under pressure and in the presence of a catalyst.

## 1220: ETHYLENEGLYCOL MONOBUTYLETHER ACETATE

*2*-Butoxyethanol acetate.
Butyl cellosolve acetate.
"Radisol".



$$\begin{array}{l} CH_2-O-C_4H_9 \\ | \\ CH_2-OOC-CH_3 \end{array}$$

$C_8H_{16}O_3 = 160.22$

Colorless liquid. Slightly soluble in water, soluble in alcohol and oils.

Weak, but pungent-warm odor, remotely reminiscent of Horseradish and Radish, or Mustard. There is no perceptible lachrymatory effect at room temperature.

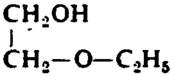
Although originally developed as an industrial solvent, this ether-acetate has been suggested for use in flavor compositions for condiments, in spice blends, etc. particularly for meat and vegetable flavoring.

It is NOT listed in the U.S. Federal Register G.R.A.S. list. The parent ether, Butyl cellosolve, is generally considered less toxic than Ethylene glycol.

Prod.: from Butanol and Ethylene chloride, using Sodium acetate as condensing agent. Subsequent Acetylation of the Glycol ether.

## 1221: ETHYLENE GLYCOL MONOETHYLETHER

Ethyl glycol (a somewhat confusing name).
Monoethyl glycol.
*2*-Ethoxy ethanol.
Cellosolve.



$$\begin{array}{l} CH_2OH \\ | \\ CH_2-O-C_2H_5 \end{array}$$

$C_4H_{10}O_2 = 90.12$

Colorless liquid. Sp.Gr. 0.93. B.P. 135° C.

Miscible with water, alcohol and most perfume oils. It is flammable but its vapors do not form explosive mixtures with air at room temperature.

Commercial grade material has a faint earthy, mushroom-like odor, but very pure analytical grades seem to be virtually odorless.

Its taste in water is bitter at concentrations of more than 50 ppm.

This very common industrial chemical is occasionally used as a solvent/diluent for perfumes, mainly for masking odors, industrial fragrances, etc., often as a co-solvent or a more or less necessary carrier/vehicle to introduce the fragrance in another type of liquid.

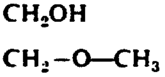
It is less toxic than Ethylene glycol, but it is banned from use in food flavors in most countries.

Prod.: from Ethanol and Ethylene chloride, heated with Sodium acetate.

31-144; 100-422; 160-978;

## 1222: ETHYLENEGLYCOL MONOMETHYL ETHER

Methyl cellosolve.
*2*-Methoxy ethanol.
Monomethyl glycol.



$$\begin{array}{l} CH_2OH \\ CH_2-O-CH_3 \end{array}$$

$C_3H_8O_2 = 76.09$

Colorless liquid. Sp.Gr. 0.97. B.P. 124° C. Flammable, and its vapors form explosive mixtures with air if the temperature is above 45° C.

Miscible with water, alcohol and most perfume oils.

Ethereal, Acetone-like odor, also resembling crude Methanol (wood alcohol).

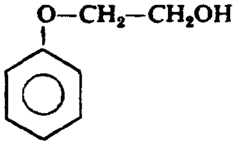
Although this industrial solvent has been suggested for use in perfumery as a solvent, the author believes that Methyl cellosolve is no longer used in perfumes or flavors. It is generally considered toxic, harmful as a liquid and as a vapor, causing considerable damage to the human CNS.

Prod.: from Methanol plus Ethylene glycol, by heating under pressure.

31-144; 100-674; 66-666;

## 1223: ETHYLENE GLYCOL MONOPHENYLETHER

Monophenyl glycol.
Phenylcellosolve.
*beta*-Hydroxyethyl phenylether.
*2*-Phenoxy ethanol.
Phenoxethol.
*1*-Hydroxy-*2*-phenoxyethane.
"Larosol".
"Arosol".
*beta*-Phenoxyethylalcohol.



$C_8H_{10}O_2 = 138.16$

Colorless liquid. Sp.Gr. 1.11. B.P. 245° C. Solidifies in the cold. M.P. 13° C.

2.7% soluble in water, soluble in aqueous alkali, miscible with Glycerin, Propylene glycol, alcohol and most perfume or flavor oils.

Mildly rosy, but also "metallic" odor of poor tenacity.

Warm mouthfeel and slightly burning taste at concentrations near 20 ppm. Higher concentrations cause more pungent feeling and bitter taste.

The title alcohol has found some use in perfume compositions as a blender, sometimes even called a "fixative". The author feels that the "fixative" value of the material is practically nil, but that it does have some blending (mellowing) effect upon certain perfume compositions containing high amounts of chemicals.

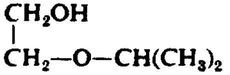
It is also used simply as a diluent of fairly harmless effect upon the odor of such (low-cost) perfumes.

Prod.: from Phenol and Ethylene oxide under alkaline conditions.

26-650; 100-798; 160-980; 163-61; 163-370; B-IV-146; 4-57;

## 1224: ETHYLENEGLOCOL MONOPROPYLETHER

Monopropyl glycol.
*2*-Propoxy ethanol.
Propyl cellosolve.
*beta*-Hydroxypropyl phenylether.
The common commercial product is the *iso*-propyl ether:



$$\begin{array}{l} CH_2OH \\ | \\ CH_2{-}O{-}CH(CH_3)_2 \end{array}$$

$C_5H_{12}O_2 = 104.15$

Colorless oily liquid. Sp.Gr. 0.91. B.P. 144° C.

Soluble in water, alcohol and most perfume oils.

Sweet, slightly spicy, vegetable, beet-like odor.

Bitter, slightly burning taste at concentrations higher than 50 ppm in water.

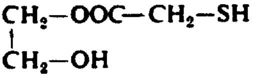
Has been used as a solvent in certain types of perfume compositions, but is more or less obsolete in perfumery now.

It is less toxic than Ethylene glycol, but – to the author's knowledge – this ether is not used in flavors.

Prod.: from Ethylene and *iso*-Propanol by heating in presence of a catalyst.

31-144; 66-666;

## 1225: ETHYLENEGLYCOL MONOTHIOGLYCOLATE



$CH_2{-}OOC{-}CH_2{-}SH$, $CH_2{-}OH$

$C_4H_8O_3S = 136.17$

Colorless, slightly viscous liquid. Sp.Gr. 1.27.

Slightly soluble in water, soluble in alcohol and oils.

The odor of this material depends largely upon the chemical purity. Minute traces of poor grade Thioglycolic acid may well impair the odor of the Monoester, while very good grades are virtually odorless.

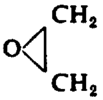
The material is mentioned mainly because it may appear as a component or as an impurity in cosmetic preparations and it is capable of altering the codor of an perfume incorporated in such funtional pyroduct significantly.

As such, the ester has little or no interest to perfumery.

34-1245; also: Ethylene glycol di-thioglycolate (see monograph).

## 1226: ETHYLENE OXIDE

*1,2*-Epoxy ethane.
Oxirane.



$C_2H_4O = 44.05$

Colorless liquid or gas. B.P. $14^{\circ}$ C.
Sp.Gr. (liquid) 0.88.

Soluble in water, alcohol and oils.

Pleasant, ethereal odor, but irritates eye and nose at high concentration of vapors.

This material finds extensive use as a fungistat in agriculture and industry. Among many other products treated, whole or ground spices may be fumigated with Ethylene oxide prior to storage to prevent mold growth during storage if the spice will not be used immediately. The permissible concentration is 15 to 50 ppm in the spice material.

As a comparison, the maximum permissible concentration of Ethylene oxide in factory working areas is 100 ppm. However, the human respiratory system may endure far higher concentrations before physical damage occurs.

G.R.A.S. F.E.M.A. No.2433.

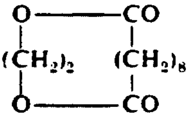
Prod.:

1) by direct oxidation of Ethylene (in this process, Formaldehyde is a normal by-product).
2) by hydrolysis of Ethylenechlorhydrin with Sodium hydroxide in aqueous solution.

31-149; 66-670; 160-994; 100-429;

## 1227: ETHYLENE SEBACATE

Glycol sebacate.
Ethylene glycol, sebacic acid, cyclic ester.
Ethylene glycol decane dioate.



$C_{12}H_{20}O_4 = 228.29$

Colorless, viscous liquid.

Insoluble in water, soluble in alcohol, miscible with perfume oils. Poorly soluble in Propylene glycol.

Sweet and very tenacious, musk-like odor with a somewhat oily undertone. Not quite as pleasant and not as strong as Ethylene brassylate.

This cyclic ester has been suggested for use in perfume compositions since its development in the late 1930's. However, it never achieved the popularity of its relative, the brassylate, developed by the same people.

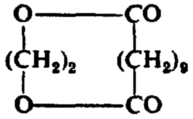
It is rarely offered commercially under its proper name, and it may not be used at all any longer.

Prod.: by esterification of Ethylene glycol with Sebacic acid under azeotropic conditions.

31-129; 86-17;
(French pat. 796410, Rhone-Poulenc) 1936.

## 1228: ETHYLENE UNDECANDIOATE

Ethylene glycol nonane dicarboxylate.



$C_{13}H_{22}O_4 = 242.32$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol, miscible with oils.

Faint, but tenacious, sweet, musk-like odor. Resembling the chemical mentioned in the previous monograph, and also Ethylene brassylate, a somewhat higher homologue, this cyclic ester has never achieved much popularity.

It is very rarely offered commercially under its proper chemical name.

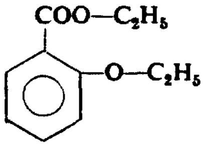
Its use would be similar to that of Ethylene brassylate.

Prod.: by esterification of Ethylene glycol with Undecan dioic acid (Homo-sebacic acid), using azeotropic conditions.

4-17; 31-129;
French patent No. 796410 (Rhone-Poulenc), 1936.

## 1229: ETHYL-beta-ETHOXY SALICYLATE

Ethyl-*ortho*-ethoxybenzoate.



$C_{11}H_{14}O_3 = 194.23$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Warm-floral, sweet and somewhat green-fruity undertone. Heavier and more fruity than Ethyl salicylate, more sweet and tenacious.

Has been suggested for use in perfume compositions, mainly in support of heavy floral notes, Ylang-Ylang, Gardenia, Hyacinth, Wistaria, etc.

This ether-ester is rarely offered under its proper chemical name, but it is used by a number of perfume houses in their special creations and bases.

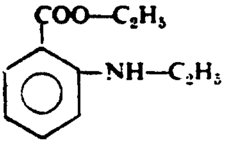
This material finds some use in flavor compositions where it may introduce interesting notes in imitation Blackcurrant, Plum, Raisin, etc. or as a part of fancy fruit complexes. It is NOT listed in the U.S. Federal Register as a G.R.A.S. material.

Prod.: by Ethylation of Ethylsalicylate, normally by way of Diethylsulfate in mild alkaline, aqueous solution and at controlled low temperature.

34-787;

## 1230: ETHYL-N-ETHYL ANTHRANILATE

"Diethyl anthranilate".
*2*-Ethylamino ethylbenzoate.



$C_{11}H_{15}NO_2$ = 193.25

Almost colorless liquid. Very poorly soluble in water, soluble in alcohol and oils. Sp.Gr. 1.12. B.P. 260 C.

Semi-dry, fruity, Grape-like, Petitgrain-like odor with a winey note.

Sweet Grape-Raisin-like taste in extreme dilution, but with a "perfumey" note.

This ester has found a little use in perfumery as a modifier where Petitgrain oil may be used, in Orangeblossom fragrances, in Honeysuckle and other sweet florals, as well as in fruity topnote complexes, bases, etc.

The ester is of little interest in flavors, since it produces more of a Petitgrain type note, less of the edible Citrus fruit notes (Grapefruit-Mandarin). In other words, it is largely outperformed by Methyl-*N*-methylanthranilate.

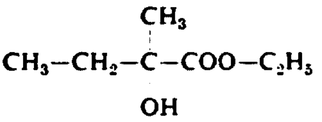
Prod.:

1) by Ethylation of Ethyl anthranilate.
2) by esterification of Ethyl alcohol with *N*-Anthranilic acid, using azeotropic conditions.
3) from *N*-Ethylisatoic anhydride with Ethanol.

34-1012; 103-164;

## 1231: ETHYL ETHYL LACTATE

*alpha*-Methyl-*alpha*-hydroxybutanoic acid, ethylester.
*alpha*-Ethyl-*alpha*-hydroxypropionic acid, ethylester.



$$CH_3-CH_2-\underset{OH}{\overset{CH_3}{C}}-COO-C_2H_5$$

$C_7H_{14}O_3$ = 146.19

Colorless liquid, slightly soluble in water, soluble in alcohol and oils.

Vinous-herbaceous odor, reminiscent of Mint and Spearmint (garden mint).

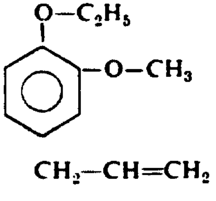
This ester belongs to a group of chemicals, developed in search of new aroma raw materials. It appears that many esters of *alpha*-hydroxy-acids have interesting odors, many have Spearmint-like odor.

This particular chemical has been suggested for use in perfumes and flavors, but it is the author's opinion that little, if any at all, of this ester is used in our industries.

31-135;
See also Ethyl methyl lactate. It is quite possible that perfumery literature includes confusion with the esters of *alpha*-ethoxypropionic acid.

## 1232: ETHYL EUGENOL

Eugenol ethylether.
*2*-Methoxy-*4*-allyl phenethole.
*1*-Ethoxy-*2*-methoxy-*4*-allylbenzene.



$C_{12}H_{16}O_2$ = 192.26

Colorless oily liquid.

Insoluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol.

Somewhat musty, but sweet-herbaceous-tealike, warm and delicately spicy odor. It is milder than Methyleugenol and less interesting as a perfume chemical. It is also less sweet and less interesting than Ethyl-*iso*-eugenol (see next monograph).

This ether has been suggested for use in perfume compositions as a modifier in Carnation fragrances, in Ylang-Ylang compositions, in Wallflower bases, and in general along with other Eugenol derivatives in warm, Oriental fragrance types. It blends particularly well with Patchouli oil, Bay leaf oil, Pimenta berry oil, etc. and creates interesting notes with Vetiver.

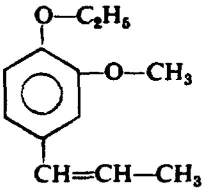
Ethyl eugenol is rarely offered commercially.

Prod.: by Ethylation of Eugenol, e.g. with Diethylsulfate in weak alkaline solution of Eugenol.

(34-1116);

## 1233: ETHYL-iso-EUGENOL

*2*-Ethoxy-*5*-propenylanisole.
*iso*-Eugenol ethylether.



$C_{12}H_{16}O_2 = 192.26$

White crystals, melting at 62° C.

Almost insoluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol.

Mild, sweet, balsamic-Carnation-like, warm and floral odor with a faintly spicy, Vanilla-like undertone.

An excellent fixative for Oriental fragrance types, modifier/fixative in Carnation bases, background in Rose compositions, and in general as a fixative with a delicate floral sweetness.

Its taste in aqueous media is quite powerful. Vanilla-like with a warm-fruity note.

This ether is used frequently in flavor compositions, particularly those which are intended for baked goods or other heat-processed foods. For imitation Vanilla, in various fruit blends as a fixative, and in spice blends, this material has great versatility and general acceptance as a flavor type.

The concentration used in candy may be as high as 15 to 20 ppm, while it is much lower in Vanilla and fruit compositions for Ice cream or baked goods.

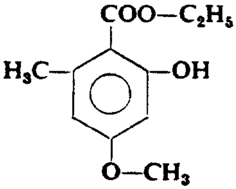
G.R.A.S. F.E.M.A. No.2472.

Prod.: by Ethylation of *iso*-Eugenol, e.g. with Diethyl sulfate and the *iso*-Eugenol in weak aqueous alkaline solution. Or: by Isomerization of Ethyl eugenol, using Potassium hydroxide in alcoholic solution under heating.

34-1116;

## 1234: ETHYL EVERNINATE

Ethyl-*2*-hydroxy-*6*-methylanisate.
*2*-Hydroxy-*4*-methoxy-*6*-methyl benzoic acid, ethylester.
or: Ethyl-*6*-hydroxy-*4*-methoxy-*ortho*-toluate.



$C_{11}H_{14}O_4 = 210.23$

White or colorless crystal needles.

Slightly soluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol.

Faint, but very tenacious odor of woody-nutlike, earthy-mossy character and a peculiar dry sweetness.

This ester is rarely offered commercially, while the Methylester is occasionally offered under the trade name "Sparassol". The two esters find use in Oakmoss compositions, in artificial Oakmoss bases, and as a type of colorless Oakmoss.

The ester presents only a modest part of the olfactory picture of Oakmoss, and it does not in any way bring the key to an artificial Oakmoss product. It blends very interestingly with Vetiver oil, and produces desirable effects with or without that oil in imitation Walnut. However, it has a certain odor character, not very often found in any chemical. But the use of this ester is accompanied by the disadvantages of a phenol, discoloration in alkaline media, sensitivity to Iron, daylight, air, etc. – the same troubles as met with in the use of Oakmoss products.

Prod.: by careful Ethylation of Everninic acid.

See literature references under: Methyl everninate.

## 1235: ETHYL FORMATE

Ethyl methanoate.
Ethyl formiate.
Formic ether.

$C_2H_5\text{—OOC—H}$

$C_3H_6O_2 = 74.08$

Colorless, mobile liquid. Sp.Gr. 0.93.
B.P. 54° C.

12% soluble in water, miscible with alcohol and oils, soluble in Propylene glycol and Glycerin. Easily hydrolyzed in presence of traces of water. The ester should be stored with a small amount of anhydrous Sodium sulfate. Pleasant, ethereal, diffusive, warm-fruity Rum-like odor.

Very flammable, and its vapors form explosive mixtures with air at room temperature.

Sweet-ethereal, fruity taste in water. Comparatively weak.

The ester finds a little use in perfumery for its effect in floral compositions (it is a natural occurrence in certain flower absolutes) and as an additive to alcohol for perfumery use to give it "lift" and "aged" notes.

It is used very extensively in flavor compositions for imitation Peach, Pineapple, Apple, Apricot, Banana, Berry, Butter, Butterscotch, Brandy, Grape, Plum, Rum, Sherry-wine, Whisky, Tutti-frutti, etc.

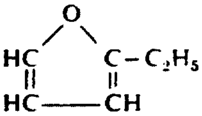
The concentration may be about 10 to 100 ppm in baked goods, and up to 450 ppm in chewing gum.

Prod.: from Glycerin, Oxalic acid and Ethyl alcohol, by heating. Also: directly from Formic acid and Ethanol.

G.R.A.S. F.E.M.A. No.2434.

31-135; 33-501; 90-194; 95-173; 96-202; 4-16; 86-17; 77-178; 26-544; B-II-19; 100-431; 103-83; 140-131;

## 1236: 2-ETHYLFURAN



$C_6H_8O = 96.13$

Colorless mobile liquid. B.P. 93 C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, sweet-ethereal, "burnt" odor, in extreme dilution rather pleasant, warm and sweet.

The title material is an empirical isomer of one of the Furanderivatives isolated from the volatile aroma of Coffee (roasted), namely *2,5*-Dimethylfuran.

This Furan is used in imitation Coffee flavor, and also occasionally in Caramel flavor. It requires considerable fixation for the latter purpose, due to the volatility of this material, while in Coffee flavor, the most volatile portion is generally the most important portion of the flavor picture.

Prod.: from Furyl methyl carbinol by dehydration, followed by reduction.

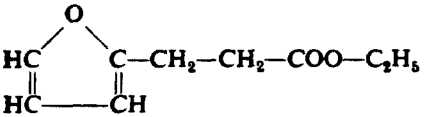
The carbinol is obtained by Grignard reaction on Furfural.

The title material is approved by the American F.D.A. as a synthetic flavor or adjuvant.

69-147; 162-629;

## 1237: ETHYL-2-FURAN PROPIONATE

Ethyl furyl propionate.
Ethyl furfuryl hydracrylate* (confusing name, see below).



$C_9H_{12}O_3$ = 168.20

Pale yellowish liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-green, slightly woody, peculiar odor, rather sharp in character, but not very powerful, mainly reminiscent of unripe fruit.

Fresh- fruity-green, somewhat sharp taste.

This ester finds use in flavor compositions for imitation Apple, Cherry, Pineapple, Raspberry, etc.

The concentration used is equivalent to a few ppm (about 2 to 10 ppm) in the finished products.

G.R.A.S. F.E.M.A. No.2435.

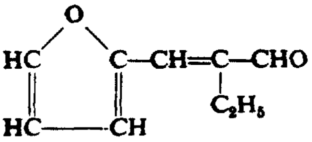
Prod.: Furanpropionic acid is prepared from Furfural via Furfuryl acrylic acid to the -hydracrylic acid. Esterification with Ethanol.

7-171;

* see also monograph: Ethyl furyl hydroxyacrylate. 4-16;

## 1238: alpha-ETHYL FURFUR ACROLEIN

*alpha*-Ethyl-*2*-furylacrolein (correct name).
*2*-Ethyl-*3*-furylacrolein.
*2*-Furfurylidene butyraldehyde.



$C_9H_{10}O_2$ = 150.18

Pale yellowish oily liquid. B.P. 240° C. Sp.Gr. 1.06.

Almost insoluble in water, soluble in alcohol and oils.

This aldehyde discolors under exposure to daylight and air.

Mild, warm-spicy, somewhat leather-like, but not medicinal or phenolic odor, slightly dry-woody, yet overall sweet. Less Cinnamon-like than the Methyl-derivative, more Labdanum-like.

Oily-fruity, sweet taste with a spicy note.

Finds occasionally use in perfume compositions accompanying Labdanum and the Eugenol derivatives in Men's fragrances, in fixative complexes for Citrus notes, and as a modifier in spicy fragrances.

The title material, which is sold under various trade names, rarely under its proper chemical name, finds some use in flavor compositions for fruit complexes, Nut flavors, Spice blends, Rum and Liqueur flavorings, etc.

The concentration is normally mere traces, about 0.5 to 6 ppm. in the finished product.

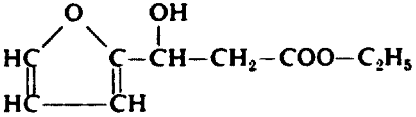
G.R.A.S. F.E.M.A. No.2492.

Prod.: by condensation of Furfural and *n*-Butyraldehyde.

31-40; 86-17;
Aetherische Oele, Riechstoffe, Parfumerien, July 1953, page 150.

## 1239: ETHYL FURFUR HYDRACRYLATE

This name is still used for a perfume and flavor chemical which – in the author's opinion – should have the correct chemical name:
Ethyl furyl hydracrylate – or:
Ethyl furyl-*beta*-hydroxypropionate.
Its structure is:



$C_9H_{12}O_4 = 184.20$

The author believes that this is the chemical, offered under the name Ethyl furfur hydracrylate.

Colorless to pale yellowish liquid, insoluble in water, soluble in alcohol and oils.

B.P. 220° C. Sp.Gr. 1.06.

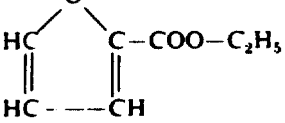
Somewhat woody, warm, Tea-like, slightly floral odor of limited tenacity.

Has been suggested for use in perfume compositions as a novel note in heavy floral perfumes, Orris compositions, Tabac-bases, Oriental fragrance types, etc.

4-16; 77-197; 4-351;
see also: Ethyl furyl hydroxy acrylate – and Ethyl-2-furan propionate.

## 1240: ETHYL FUROATE

Ethyl-2-furan carboxylate.
Ethyl furan-*alpha*-carboxylate.
Ethyl pyromucate.



$C_7H_8O_3 = 140.14$

White leafy or prismatic crystals. M.P. 34° C. Sp.Gr. 1.09 (liquid). B.P. 195° C.

Insoluble in water, soluble in alcohol and oils.

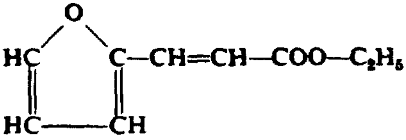
Warm, fruity-floral odor slightly more pungent than that of Ethyl benzoate. There are very pleasant "overripe fruit" or Plum-Raisin-like undertones. This ester has been suggested for use in flavor compositions, mainly in berry flavor imitations, Grape, Wine, etc. However, this material is NOT included in the G.R.A.S. list of the U.S. Federal Register.

Prod.: from Furfural by oxidation to 2-Furoic acid, followed by esterification.

7-171; 8-465; 31-127; 69-157; 100-431; 160-1008; B-XVIII-275; 26-544; 140-174;

## 1241: alpha-ETHYL FURYL ACRYLATE

*cis-* and *trans-*forms are known.



$C_9H_{10}O_3$ = 166.18

Yellowish liquid. B.P. 230° C.

Insoluble in water, soluble in alcohol and oils.

Sweet-balsamic, floral odor of modest tenacity.

Has been suggested for use in perfume and flavor compositions, but the author believes that this ester is only very rarely, if ever, used in perfumes.

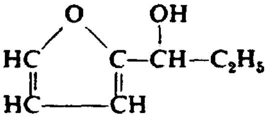
It finds some use in flavors for imitation Maple, Coffee, Caramel, Walnut, Rum, etc.

Prod.: from Furfural.

69-159; 86-17;

## 1242: ETHYL-2-FURYL CARBINOL

Ethyl furfuryl alcohol.
2-Furyl ethyl carbinol.



$C_7H_{10}O_2$ = 126.16

Colorless liquid. B.P. 170° C.

Slightly soluble in water, soluble in alcohol and oils.

Warm-caramellic, sweet and somewhat floral odor.

Burning, yet rather sweet caramellic-floral taste.

Has been suggested for use in flavor compositions.

However, the flavor type and the character of this material does not seem to be very unusual or in any way superior to the conventional caramellic-fruity-floral flavor materials of recent date of origin.

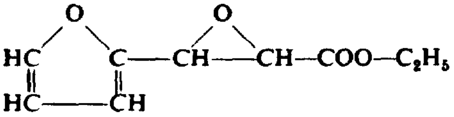
It is very rarely offered commercially.

Prod. from Furfural by Grignard type reaction.

69-151;

## 1243: ETHYL FURYL GLYCIDATE

Ethyl-*beta*-furyl glycidate.
*beta*-2-Furyl-*alpha*-*beta*-epoxy ethylpropionate.



$C_8H_{10}O_4$ = 170.17

Colorless to pale straw-colored, slightly viscous liquid. Almost insoluble in water, soluble in alcohol and oils.

Sweet-fruity, warm-caramellic, somewhat "burnt" odor of moderate tenacity.

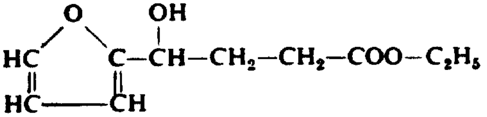
Sweet-fruity, "jam"-like taste, remotely reminiscent of cooked Strawberries.

Could find some use in flavor compositions as a modifier for Ethyl phenyl glycidate, which is somewhat more floral-fruity, but there has not been much interest in the subject ester.

Prod.: from Furfural and Ethyl monochloro acetate by condensation using a catalyst.

## 1244: *ETHYL FURYL HYDROXY ACRYLATE

Ethyl furfuryl ethylene lactate.
* correct name for Ethyl furfuryl hydracrylate.



$C_{10}H_{14}O_4 = 198.22$

This is the chemical, with which Ethyl furfuryl hydracrylate is often confused.

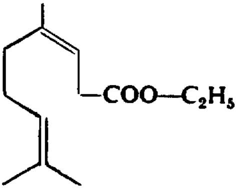
The subject chemical is not known to the author as a perfume or flavor material and may not be such type of material.

It is mentioned here for the completion of the "furacrylate" series in flavor and perfume literature.

B-III-295;
see also: Ethyl furfur hydracrylate and: Ethyl -*2*-furan propionate.

## 1245: ETHYL GERANATE

Ethyl geraniate.
Ethyl-*3*,*7*-dimethyl-*2*,*6* (and *2*,*7*)-octadienoate.



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Mild, woody-rosy, somewhat green odor.

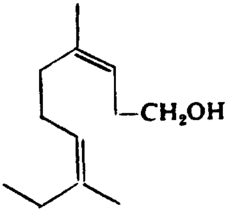
This chemical has been produced by a few manufacturers mostly for the purpose of introducing the material in artificial oils and special fragrance bases. Its use in conventional creative perfumery is very limited.

Prod.: from Ethoxy acetylene plus Ethyl Magnesium Bromide with Methylheptenone, followed by acidification with diluted sulfuric acid.

90-136;

## 1246: ETHYL GERANIOL

"Homogeraniol".
The commercial product, when available, usually contains substantial amounts of Ethyl citronellol, see that monograph.
Mainly: *2*-*trans*-*3*,*7*-Dimethyl-*2*,*6*-nonadien-*1*-ol.



$C_{11}H_{20}O = 168.28$

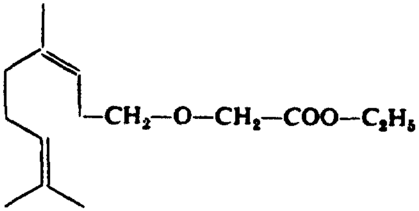
Colorless to pale yellowish liquid, almost insoluble in water, soluble in alcohol, miscible with most oils.

The odor is fattier and less woody than that of Geraniol, but since the commercial product is far from pure, it is not possible to give more than an approximate odor description.

This material has found very little interest among creative perfumers.

## 1247: ETHYL GERANOXY ACETATE

Geranoxyacetic acid, ethylester.



$C_{14}H_{24}O_3 = 240.35$

Colorless oily liquid. B.P. 262° C.

Insoluble in water, soluble in alcohol, miscible with most oils.

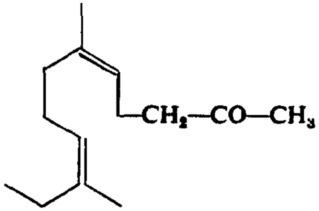
Slightly rosy, sweet and delicately musky odor. Some observers find the odor so weak, that it is classified as "musky" just for that reason. However, it has considerable odor value, clearly displayed when this material is blended with more volatile components.

Has been suggested for use in perfume compositions as a fixative and modifier in rose perfumes, sweet-floral bases, etc. It is very rarely offered commercially, and has therefore never become well known or popular.

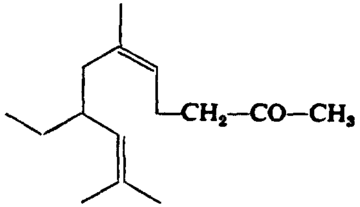
31-158;

## 1248: ETHYL GERANYL ACETONE

"Homogeranyl acetone".
The commercial product is:
*6,10*-Dimethyldodecadien-*5,9*-one-*2*.
True Ethylgeranylacetone is *6*-Ethyl geranyl acetone. Its structure is given below with the structure for commercial EGA.



Commercial product



"True" E.G.A.

$C_{14}H_{24}O = 208.35$

Colorless or pale straw-colored oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-floral, fruity, soft and warm odor of fair to good tenacity.

This ketone has found some use in perfume compositions, mainly better soap perfumes. Its stability and rich power are welcome improvements over many conventional perfume chemicals of similar odor type. The main drawback is its relatively high cost (for the purposes mentioned) which is a very common drawback for new aromatic chemicals – and usually only overcome in case of unquestionable success of the fragrance performance of the material. The initial cost of developing, manufacturing and marketing a new aromatic chemical will normally be calculated into the initial price of the material. The result is most often a shock to the prospective customer. Only very well established and solidly founded companies can afford to carry these initial expenses in such a way that the new chemical is marketed at an extremely attractive price from the very beginning. On the other hand, a quick increase in sales may enable the manufacturer to initiate large-scale batch-making much sooner than expected, so that manufacturing cost is quickly reduced and the selling price is in reasonable proportion to the cost of large-scale production.

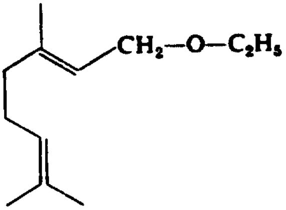
Prod.: from Ethyl linalool with Ethylacetoacetate and Sodium ethylate.

Sample: Hoffmann-laRoche, Inc.

See also: Geranyl acetone.

## 1249: ETHYL GERANYL ETHER

Geranyl ethyl ether.
Do not confuse with Ethyl geraniol (Ethyl citronellol).



$C_{12}H_{22}O = 182.31$

Colorless oily liquid. B.P. 214° C. Sp.Gr. 0.87.

Insoluble in water, soluble in alcohol, miscible with oils.

Diffusive-green, fresh-leafy, somewhat grassy and sweet odor of moderate tenacity. The greenness tends to be vegetable-like, sometimes described as "lettuce-juice"-like, while the sweetness is almost floral.

This ether has been suggested for use in perfume compositions, particularly in soap perfumes, since it is stable in mild alkali. Various literature sources state that the odor of the ether is too weak to warrant any further use of the material, but it is most conceivable that such odor descriptions are based upon study of impure material, or unidentified material. The odor is definitely more powerful than that of Geraniol, and it has an entirely novel type of greenness and freshness.

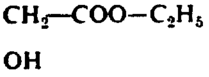
Subject ether should have good possibilities of application in perfumery and soap perfumery. It lends power and freshness to a Lavandin composition, lift to a Geranium, and natural greenness to the modern "outdoor" type fragrances for room sprays, etc.

Prod.: (several methods), e.g. from Geranyl chloride plus Sodium ethoxide in Ethyl alcohol. Also from Linalool by isomerization under ethylalcoholic conditions.

5-19; 86-55;

## 1250: ETHYL GLYCOLATE

Ethyl hydroxy acetate.
Ethyl hydroxy ethanoate.



$$\underset{OH}{CH_2}—COO—C_2H_5$$

$C_4H_8O_3 = 104.11$

Colorless liquid. Sp.Gr. 1.08. B.P. 160° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar ethereal, weedy-winey odor, often classified as "Spearmint-like".

The corresponding acid occurs in unripe Grapes.

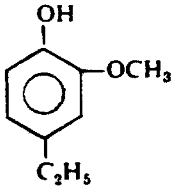
The ester has been suggested for use in flavor compositions, but the author is unaware of its use in any type of flavor.

Prod.: from Ethylene glycol by oxidation to Glycollic acid, followed by esterification.

31-135; 66-784; 160-1020;

## 1251: 4-ETHYL GUAIACOL

Do NOT confuse with: Guaiacol ethylether.
*2*-Methoxy-*4*-ethylphenol.
Homocreosol.
*1*-Hydroxy-*2*-methoxy-*4*-ethylbenzene.



$C_9H_{12}O_2 = 152.20$

Almost colorless, oily liquid, solidifying in the cold. M.P. 11° C. B.P. 234° C. Sp.Gr. 1.06.

Poorly soluble in water, soluble in alcohol and miscible with most oils.

Warm, sweet and spicy-medicinal, very powerful odor, reminiscent of Guaiacol and Eugenol at the same time. The odor is extremely diffusive and penetrating.

Apart from very occasional use in perfumery, this material finds use in flavor compositions for imitation Coffee and fruit flavors. The concentration used is always mere traces, usually equivalent to 0.05 to 1.0 ppm in the functional product.

Although this material is mainly consumed in aqueous media, it is apparently its odor, not so much its flavor, that influences the aroma of the end product. There is only a very slight Vanilla sweetness in the flavor while the odor is the dominant factor.

Prod.:

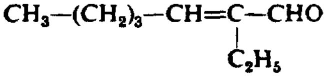
1) from *ortho*-Dichloro ethylphenol by heating with Ethyl benzyl disulfonic acid and aqueous alkali at 180-200° C, followed by single Methylation.
2) by oxidation of *para*-Ethyl salicylic aldehyde with alkaline Hydrogen peroxide, followed by single Methylation.

G.R.A.S. F.E.M.A. No.2436.

90-391;

## 1252: 2-ETHYL-2-HEPTENAL

*2*-Ethyl-*3*-butylacrolein.
"*iso*-Nonenoic aldehyde".



$CH_3{-}(CH_2)_3{-}CH{=}\underset{C_2H_5}{\underset{|}{C}}{-}CHO$

$C_9H_{16}O = 140.23$

Colorless mobile liquid. Almost insoluble in water, soluble in alcohol, miscible with oils, fairly soluble in Propylene glycol.

Very powerful, sharp-green, but refreshing odor (in high dilution) with a nut-like undertone, oily but not truly fatty.

In dilutions of less than 2 ppm, the taste in aqueous media is refreshingly green-fruity, sweet-nutlike, yet somewhat sharp. The nutlike note is sometimes described as "woody", but the author of this work finds that it is characteristically sweet and resembles Coconut and Hazelnut more than it does any type of wood.

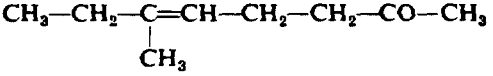
This unsaturated Aldehyde is used in flavor compositions, almost exclusively in Pineapple flavors as a trace component in amounts equivalent to 0.03 to 2 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2438.

Prod.: by condensation of *n*-Valeric aldehyde with *n*-Butyric aldehyde.

## 1253: ETHYL HEPTENONE

*6*-Methylocten-*5*-one-*2*.
Methyl ethyl hexenone.



$CH_3{-}CH_2{-}\underset{CH_3}{\underset{|}{C}}{=}CH{-}CH_2{-}CH_2{-}CO{-}CH_3$

$C_9H_{16}O = 140.23$

Pale straw-colored or almost colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful green, fatty-oily, citrusy, Bitter-Orange-like odor, softer and less harsh than Methyl heptenone.

Suggested for use in perfume compositions. Particularly suitable for creation of fresh top-note compositions with Citrus oils, best with low-terpene-, or terpeneless oils. It blends well with Citral, Linalool, Tetrahydrolinalool, Dihydrolinalool, and other fresh floral-citrusy notes. Its topnote character falls well into a Chypre picture or a conventional Citrus cologne type.

(Hoffmann-laRoche, sample).

Prod.: From Methyl ethyl ketone and Acetylene via Ethyl butynol to Ethyl butenol. This ketone is treated with Aceto acetic ester in presence of Aluminium propoxide to yield Ethyl heptenone. The subject ketone is an intermediate in the preparation of Ethyl linalool. (See that monograph).

## 1254: ETHYL HEPTIN CARBONATE

Ethyl-2-octynoate.

$CH_3(CH_2)_4C{\equiv}C{-}COO{-}C_2H_5$

$C_{10}H_{16}O_2 = 168.24$

Almost colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils. B.P. 220° C. Sp.Gr. 0.93.

Powerful foliage odor with pleasant oily-waxy undertone. The green note is somewhat Violet-leaf-like, yet sweeter and waxier than the odor of Methyl heptin carbonate.

Suggested for use in perfume compositions, particularly where a green note is part of a floral complex: Cassie, Mimosa, Violet, Lilac, Narcisse, Tuberose, etc. and in imitation "Cucumber" odors.

It has been claimed that the Ethylester is more stable in soap than the Methylester. However, the Ethylester is comparatively rare in the perfumery trade, and the Methylesters are still the most common ones.

Prod.: from Castor oil via Ricinoleic acid to Heptyne (which is now a commercially available intermediate). The Heptyne is transformed into its Sodio-derivative which is treated with Ethyl chlorocarbonate to yield Ethyl heptin carbonate. Other methods are also used.

4-16; 5-241; 7-171; 96-216;

## 1255: ETHYL HEPTOATE

Ethyl heptylate.

Ethyl-*n*-heptanoate.

Note: See also monograph on: Ethyl oenanthate, a name often used for Ethyl heptoate (and vice versa), causing some confusion.

$CH_3(CH_2)_5COO{-}C_2H_5$

$C_9H_{18}O_2 = 158.24$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 189° C.

Insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful, fruity-wine-like, Brandy- and Berry-like odor with an oily-sharp undertone.

Fruity and fermentation-winey taste, Brandy-Berry-like with a warm, somewhat sharp or acrid aftertaste, unless highly diluted.

Not quite as sweet as Ethyl nonylate, and not as rich as Ethyl oenanthate (mixed esters, see monograph: Ethyl oenanthate).

Finds some use in perfumery, particularly for topnote effects in fresh-fruity, citrusy odors, and as a "rapid-ageing" agent for alcohol, used in perfume or Cologne solutions. It imparts at trace level a pleasant "round and mellow" character to alcohol, resembling the effect of true ageing of the alcohol or its solutions.

Very extensively used in flavor compositions for imitation Butter, Butterscotch, Apple, Coffee, Cheese, Apricot, Currant, Brandy, Cocoa, Blackberry, Gooseberry, Coconut, Grape, Cognac, Malt, Nut, Tea, Rum, Quince, Melon, Peach, Plum, Pineapple, Vanilla, etc. etc. – one of the most widely used of all the common esters.

Concentrations are about 300 to 400 ppm in Gelatins and Puddings, often lower in soft drinks, hard candy and candy, higher in chewing gum.

G.R.A.S. F.E.M.A. No.2437.

Prod.: by direct esterification of Ethanol with *n*-Heptanoic acid using azeotropic condition. The ester forms an azeotrop with water, boiling at less than 100° C and containing about 75% ester, 25% water.

4-16; 33-501; 34-806; 35-61; 77-187; 86-18; 100-434; 103-91; 160-968; 26-548; B-II-340; 140-142;

NOTE: see monograph: Ethyl oenanthate.

## 1256: ETHYL HEPTYL ETHER

Heptyl ethyl ether.
*3*-Oxanonane.

$CH_3{-}CH_2{-}O{-}CH_2(CH_2)_5CH_3$

$C_9H_{20}O = 144.26$

Colorless liquid. B.P. 165° C. Sp.Gr. 0.79.

Insoluble in water, soluble in alcohol and oils.

Oily-green, somewhat harsh-fruity, sharp odor, reminiscent of unripe berries.

To the best of the author's knowledge, this ether is rarely, if ever, used in perfume compositions.

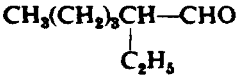
It finds some use in flavor compositions in imitation fruit and berry flavors, where it introduces fruity-green nuances and great power. Its taste in aqueous media is not quite sweet.

Prod.: from *n*-Heptyl bromide plus Sodium ethoxide in ethylalcoholic solution and in presence of a catalyst.

4-16; 37-176;

## 1257: 2-ETHYL HEXANAL

"*iso*-Caprylic aldehyde".
*iso*-Aldehyde C-8.
Butyl ethyl acetaldehyde.
*alpha*-Ethyl caproic aldehyde.
*alpha*-Ethyl hexanal.



$$CH_3(CH_2)_3\underset{\substack{|\\ C_2H_5}}{CH}{-}CHO$$

$C_8H_{16}O = 128.22$

Colorless mobile liquid. Poorly soluble in water, soluble in alcohol and oils, fairly soluble in Propylene glycol.

Comparatively mild, fruity odor, less fatty than *n*-Octyl aldehyde, and lacking the "rancid" type odor of that aldehyde.

Powerful fruity-floral taste in high dilution.

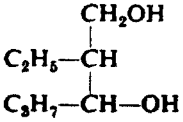
This aldehyde, normally manufactured by industries other than the perfume industry, has been suggested for use in perfumes and flavors. It does not seem to have found much usage so far, but it could be interesting in Citrus topnote complexes, in fresh floral fragrances, as a topnote component in Chypres, etc., and in flavor compositions such as imitation Banana, Peach, Apricot, etc.

Prod.: by oxidation of *2*-Ethyl hexanol, which is manufactured industrially on a large scale.

86-18;

## 1258: ETHYL HEXANE DIOL

"Rutgers 6-12".
*2*-Ethylhexanediol-(*1*,*3*).
Ethyl hexylene glycol.
*2*-Ethyl-*3*-propyl-*1*,*3*-propanediol.



$$\begin{array}{l} \qquad\quad CH_2OH \\ \qquad\qquad | \\ C_2H_5{-}CH \\ \qquad\qquad | \\ C_3H_7{-}CH{-}OH \end{array}$$

$C_8H_{18}O_2 = 146.23$

Colorless oily liquid. Sp.Gr. 0.94.
B.P. 244° C.

4% soluble in water, miscible with alcohol and oils. The glycol will absorb up to 11% water.

Peculiar "Witch-Hazel"-like odor, more often described as "musty" slightly earthy, overall weak.

This material is very rarely, if ever, used as an active ingredient in perfume or flavor compositions. It does serve, however, at times, as a solvent or diluent.

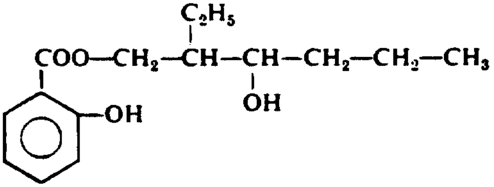
This glycol is one of the most commonly used insect (mosquito)-repellants, and since it is used at rather high concentration in the functional product, it will influence the odor of most perfumes used in the consumer product.

It has a bitter taste at concentrations higher than 50 ppm.

Prod.: from *n*-Butyric aldehyde and Magnesium Aluminum Ethoxide followed by hydrolysis of the resulting Ethyl hexyl butyrate.

100-431;

## 1259: 2-ETHYLHEXANE-1,3-DIOL MONOSALICYLATE



$C_{15}H_{22}O_4 = 266.34$

Colorless viscous liquid.

Very slightly soluble in water, slightly soluble in cold alcohol, soluble in warm alcohol and in most oils.

Musty odor, often described as "Witch-Hazel"-like, a description used about quite a number of higher glycols and glycol esters, therefore possibly referring to (unknown) impurities in commercial grades of glycols.

The title material has found some use as a sunscreening agent in cosmetic preparations, and the author has no report of its being used in perfumes as an active olfactory ingredient.

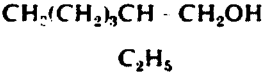
It is briefly mentioned here because it may be used at high concentration in the functional product (up to 20 or 50 times the conventional perfume level in same type product). It is therefore important to study the odor of such materials in order to be able to efficiently perfume them.

*2*-Ethyl-*1,3*-hexanediol is a common Glycol, made in large volume as an industrial chemical. It has B.P. 243° C. Sp.Gr. 0.94 and is soluble at the rate of 4% in water.

## 1260: 2-ETHYL HEXANOL

*2*-Ethyl hexyl alcohol.

NOTE: The name "Capryl alcohol" is sometimes used for this alcohol. The material, listed in this work under the name: OCTANOL-*1*, is most commonly called "Capryl alcohol".



$$CH_3(CH_2)_3\underset{\displaystyle C_2H_5}{CH}-CH_2OH$$

$C_8H_{18}O = 130.23$

Colorless oily liquid. Sp.Gr. 0.83.
B.P. 185° C.

0.15% soluble in water. The material will dissolve 2½% water. Soluble in alcohol and oils.

Comparatively mild, oily, sweet and slightly floral-rosy odor. Sweet, fatty-floral taste with a fruity note.

Mainly serving as an intermediate in making perfume and flavor chemicals, this material is occasionally used in perfumes for masking and for other industrial purposes. It is an inexpensive chemical and blends well with the powerful floral and fruity materials conventionally used in masking compositions.

Prod.: by way of petrochemical synthesis.

29-476; 100-743; 160-1034;

## 1261: ETHYL HEXIN CARBONATE

Ethyl heptynoate.
Ethyl-*n*-hex-*1*-yne carboxylate.

$CH_3(CH_2)_3C{\equiv}C{-}COO{-}C_2H_5$

$C_9H_{14}O_2 = 154.21$

Colorless oily liquid. B.P. 201° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful leafy-green odor of moderate to poor tenacity. Less gassy and less pungent than Methyl heptin carbonate, but not as fresh-leafy as Methyl hexin carbonate.

This ester is another member of a very long series of acetylenic esters developed in search of more natural or interesting smelling esters to accompany or substitute Methyl heptin carbonate, one of the better known members of the series.

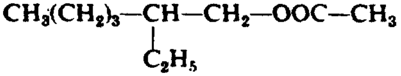
Very rarely offered under its proper chemical name, it has been offered as component of mixtures of several acetylenic esters in specialties or perfume bases. The commercial availability of a very extensive series of Hexenyl esters has largely made the acetylenic esters uninteresting, in many cases making them obsolete, particularly since there is no economical advantage in the use of the acetylenic esters.

Prod.: from Methyl-*n*-butylketone via *n*-Hex-*1*-yne to the acid from which the Ethylester is prepared.

5-245;

## 1262: 2-ETHYL HEXYL ACETATE

*beta*-Ethyl hexyl acetate.
"*iso*-Octylacetate".
*2*-Ethyl hexanyl acetate.



$$CH_3(CH_2)_3{-}\underset{\displaystyle C_2H_5}{\underset{|}{CH}}{-}CH_2{-}OOC{-}CH_3$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Sp.Gr. 0.87. B.P. 199° C.

0.01 % soluble in water, soluble in alcohol and oils.

Very pleasant, sweet-fruity odor reminiscent of Raspberry juice, sweeter than Octyl acetate and free from its herbal notes.

Subject ester has found some use in perfumery, mainly in soap perfumes, since it is comparatively stable in alkali and blends well with the fruity-floral materials, used in low-cost coaps and detergents.

Ethyl hexyl acetate finds use in flavor compositions for its powerful fruity and comparatively lasting freshness, overall more agreeable than Benzyl acetate and Amyl acetate. It finds use in certain types of imitation Raspberry and berry complexes, e.g. for hard candy flavors.

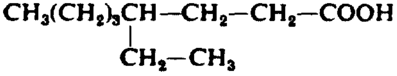
Prod.: by direct esterification of *2*-Ethyl hexanol with Acetic acid under azeotropic conditions, or with Acetic anhydride.

31-122; 160-1034;

## 1263: 2-ETHYL HEXYL ACETIC ACID

- * Perfumery literature has shown cases of confusion with *2*-Ethylhexanoic acid, which is more commonly used in preparation of flavor esters, etc.

The title material represents an *iso*-Decanoic acid:



$$CH_3(CH_2)_3\underset{\displaystyle CH_2{-}CH_3}{\underset{|}{CH}}{-}CH_2{-}CH_2{-}COOH$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid, solidifying in the cold to a waxy mass.

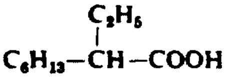
Practically insoluble in water, soluble in alcohol and oils.

Relatively weak, fatty-acrid odor of considerable tenacity. Less nutty, more fruity than Decanoic acid.

This acid has been suggested for use in flavor compositions, mainly in Cheese and Butter compositions, as a modifier for the conventional fatty acids.

It is rarely offered commercially, and it does not appear to have much importance as a flavor ingredient.

- 2-Ethyl-2-hexyl acetic acid is also known and has been reported in literature in connection with the title mtaerial. It has the following structure:

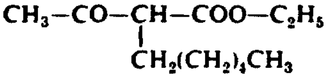


$$C_6H_{13}-\overset{\overset{\displaystyle C_2H_5}{|}}{C}H-COOH$$

and it is derived from 2-Hexylbutanol-*1*.

## 1264: ETHYL-2-HEXYL ACETOACETATE

Hexyl acetoacetic ester.



$$CH_3-CO-\underset{\underset{\displaystyle CH_2(CH_2)_4CH_3}{|}}{C}H-COO-C_2H_5$$

$C_{12}H_{22}O_3 = 214.31$

Colorless slightly oily liquid. Very slightly soluble in water, soluble in alcohol, miscible with oils.

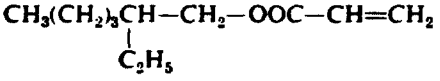
Oily-herbaceous, somewhat winey odor with distinctly green-herbal notes, reminiscent of undertones in Jasmin complex.

This ester has found some use in perfume compositions, mainly as an ingredient in Jasmin bases, occasionally in other floral bases where the green-winey-herbaceous and fresh ethereal note may be desirable.

Prod.: by condensation of Ethyl acetate and Hexyl acetate, using Sodium ethoxide catalyst.

## 1265: 2-ETHYL HEXYL ACRYLATE

*iso*-Octyl acrylate.
*3*-Octanyl propenoate.



$$CH_3(CH_2)_3\underset{\underset{\displaystyle C_2H_5}{|}}{C}H-CH_2-OOC-CH{=}CH_2$$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. B.P. 216° C. 0.88.

0.1% soluble in water, miscible with alcohol and oils.

Powerful and diffusive, sweet-herbaceous, balsamic odor with a mildly "gassy" character (often found in acrylates, etc.).

This ester has been suggested for use in artificial essential oils, and it was commercially available at a very low cost during an early period of perfume chemical development, before the more desirable members of related series were developed.

It was therefore used in certain perfume types to support and emphasize warm-herbaceous notes, to give lift to Lavender/Coriander, Labdanum, and to give Chamomile-like effects in topnote compositions.

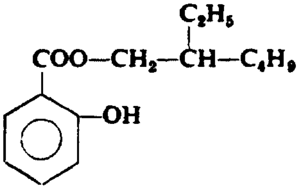
The title ester has long since been outperformed by other and "safer" perfume chemicals, and it is probably very rarely used today.

Prod.: by esterification of 2-Ethylhexanol with Acrylic acid. The commercial product usually contains an inhibitor to retard polymerization (Hydroquinone or other).

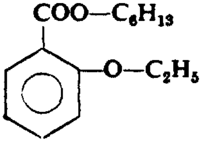
Info.: Dow Chemical Company, Midland, Mich., U.S.A.

## 1266: ETHYL HEXYL SALICYLATE

**Salicylic acid, *2*-Ethylhexanoic ester.**
**Confusion with *ortho*-Ethoxy hexylbenzoate* has occurred in literature.**



Ethyl hexyl salicylate
(Title material)



*) *ortho*-Ethoxy hexyl salicylate

$C_{15}H_{22}O_3 = 250.34$
(both materials)

**Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.**

Heavy, fruity, slightly spicy-floral odor of moderate tenacity.

Blackcurrant-type, heavy fruity flavor, but pleasant only at concentrations lower than 20 ppm.

This ester, rarely offered commercially, has been used in perfumes and flavors as a modifier for Methyl benzoate, Ethyl benzoate, Ethyl salicylate and similar esters for floral-spicy effects in fragrances or for Blackcurrant-Cherry type flavors.

The ester is not listed in the American Federal Register or in the G.R.A.S. list of the F.E.M.A. It should therefore be considered as banned from food flavors in the U.S.A.

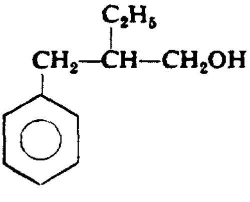
Prod.: from *2*-Ethylhexanol and Salicylic acid by azeotropic type esterification.

* *ortho*-Ethoxy hexylsalicylate is prepared from Hexylsalicylate by Ethylation with Diethylsulfate.

4-16; 34-787;

## 1267: alpha-ETHYL HYDROCINNAMIC ALCOHOL

*alpha*-Ethyl-*beta*-phenyl propanol.



$C_{11}H_{16}O = 164.25$

Almost colorless oily liquid. B.P. 242° C.
Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils.

Mild clover-like, somewhat musky-sweet, tenacious odor.

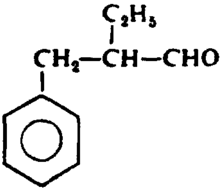
Has been suggested for use in perfumery as a modifier for the more odorous members of this chemical series, but there has been very little interest in this alcohol.

Prod. by careful selective reduction of *alpha*-Ethyl cinnamic aldehyde.

93-151;

## 1268: alpha-ETHYL HYDROCINNAMIC ALDEHYDE

*2*-Ethyl-*beta*-phenylpropionic aldehyde.



$C_{11}H_{14}O = 162.23$

Almost colorless oily liquid. B.P. 231° C. Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Pleasant, mild odor, warm and sweet, slightly cinnamic, mainly balsamic.

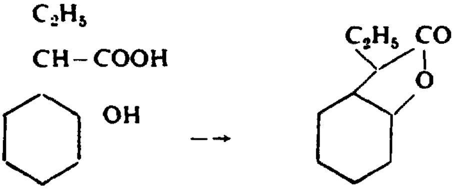
Has been suggested for use in perfume compositions, but does not seem to have achieved much popularity.

This aldehyde is rarely offered commercially.

Prod.: by hydrogenation of *alpha*-Ethyl cinnamic aldehyde. The alcohol and other saturated compounds are formed at the same time.

30-246; 31-37; 93-152;

## 1269: alpha-ETHYL-2-HYDROXY CYCLOHEXANEACETIC ACID, gamma-LACTONE



Parent acid see below*) Lactone

$C_{10}H_{16}O_2 = 168.24$

Colorless viscous oil. Almost insoluble in water, soluble in alcohol, miscible with oils, very poorly soluble in Propylene glycol.

Woody-coumarinic, somewhat weedy-Cedarleafy odor with an overall "Bittersweet" character and good tenacity.

Bitter-woody taste in water at concentrations above 10 ppm.

This lactone, remotely related to Coumarin (or rather to a *3*-substituted Hydrocoumarin with one Methylene-linkage less than Hydrocoumarin) has been suggested for use in perfumery for its powerful Coumarin-like character, sometimes described as more Tonka-like than Coumarin itself.

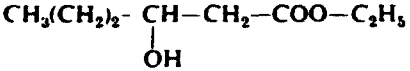
However, in spite of its power, it does not possess the softness found in ordinary alkyl-substituted Coumarins, which can be used at widely varied concentrations. The subject lactone is easily overdosed and may cause sharp, bitter effect.

It performs excellently in soap, but it has the same chemical drawbacks as the other lactones – sensitivity to alkali, etc.

Prod.: by Lactonization of the hydrogenated, *alpha*-ethyl-substituted *ortho*-hydroxy-Phenylacetic acid.*

## 1270: ETHYL-3-HYDROXY HEXANOATE

Ethyl-*3*-hydroxycaproate.



$CH_3(CH_2)_2\text{-}\underset{OH}{CH}-CH_2-COO-C_2H_5$

$C_8H_{16}O_3 = 160.22$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.

Powerful, fresh-fruity-oily, slightly green odor.

Fresh-fruity, light and powerful, penetrating taste.

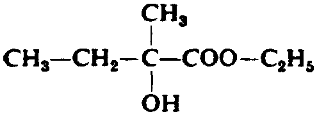
This ester has been suggested for use in flavor compositions, mainly in Citrus type flavors. It is also used to reconstitute the natural type flavor in Orange juice.

Prod.: by esterification of *beta*-Hydroxy caproic acid, which is an isomer of Leucic acid. The acid can be obtained from Butyraldehyde by condensation with Bromo acetic ester in presence of Zinc catalyst.

(Journal of Food Science, 29, 790 (1964).

## 1271: ETHYL-alpha-HYDROXY-alpha-METHYLBUTYRATE

*2*-Hydroxybutane-*2*-carboxylic acid, Ethylester.
Methylethylglycollic acid, Ethylester.



$$CH_3{-}CH_2{-}\overset{\overset{\textstyle CH_3}{|}}{\underset{\underset{\textstyle OH}{|}}{C}}{-}COO{-}C_2H_5$$

$C_7H_{14}O_3 = 146.19$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Fruity, herbaceous-sweet and overall refreshing odor of moderate to poor tenacity. The fruity notes are rather diffusive, the herbaceous notes are warm, slightly spicy or rooty.

This ester has been suggested for use in perfume compositions as a modifier in modern herbaceous fragrances, including Lavender/Lavandin, Clary Sage, etc. in Colognes or Citrus-compositions for topnote bases, and in general in novel fragrance types for household products, etc.

The raw material is very inexpensive, and the title ester can be manufactured at a very attractive cost, but it has not succeeded in "breaking the ice" with the perfumer. Most perfume laboratories are without it, and the material is not often offered since it mostly comes from manufacturers other than those who make perfume chemicals.

Prod.:

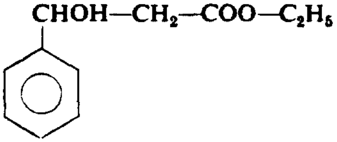
1) from Ethyloxalate with Zinc, Methyl iodide and Ethyliodide.
2) from Methyl ethyl ketone via its Cyanhydrin and by hydrolysis to the Glycollic acid. Ethyl-esterification yields the title material.

Method No. 2) is the common commercial method.

66-781; 66-787;

## 1272: ETHYL-3-HYDROXY-3-PHENYLPROPIONATE

*2*-Phenyl-*2*-hydroxy ethylpropionate.
Dihydro-ethylbenzoyl acetate.



$C_{11}H_{14}O_3 = 194.23$

Colorless or very pale straw-colored oil. Almost insoluble in water, soluble in alcohol and oils.

Sweet-balsamic, fruity and slightly floral, herbaceous, warm odor, reminiscent of the most pleasant notes in refined Labdanum products.

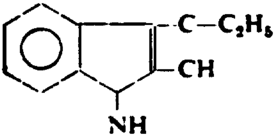
This ester is used in perfumery to emphasize Labdanum and Ambrenotes, particularly where it may be essential that color is kept at a minimum. The ester is not as stable in soap as Labdanum itself, but it performs well in Fougeres, Oriental bases, Chypres, etc. for general cosmetic perfumery.

Prod.: by hydrogenation of Ethyl benzoyl acetate. This parent material is obtained by condensation of Acetophenone with Ethyl carbonate.

See also: Ethyl benzyl acetoacetate, and
Ethyl benzoyl acetate.

## 1273: beta-ETHYL INDOLE

Homo skatole.



$C_{10}H_{11}N = 145.21$

White crystals, melting at 37° C. B.P. 252°C. Crystals darken upon exposure to daylight.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Powerful animal-tarry odor, in extreme dilution sweet and floral, somewhat animal, but not at all faecal. Very tenacious.

This higher homologue of Skatole has been suggested for use in perfume compositions, mainly in special bases, animal-type bases, heavy floral bases, etc. partly as a modifier for Skatole, partly as a more versatile item, since it lacks the unpleasantly faecal notes of Skatole.

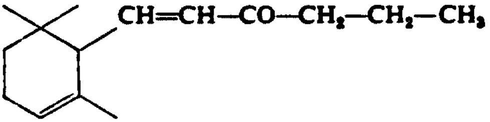
A very rare perfume chemical.

Prod.: from Indole with Sodium ethoxide in Ethanol under pressure and heat.

5-313;
See also: Dimethyl indole.

## 1274: alpha-ETHYL IONONE

*6*-(*2*,*6*,*6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*5*-hexen-*4*-one.
See also: Cyclocitrylidene methylbutanone.
Commercial products contain several isomers. The above name and the structure below refer to the *alpha*-isomer.



$C_{15}H_{24}O = 220.36$

Pale straw-colored, yellowish or almost colorless oil. B.P. 259° C.

Pleasant, warm-woody, powdery type odor.

See comments about odor description of Ionones under Cyclocitrylidene methylpentanone.

This higher homologue of Methylionone finds use in perfume compositions as a modifier for the conventional isomers of Methylionone, mainly because of its slightly superior tenacity and more powdery character. It appears on the market almost exclusively under trade names.

Prod.: by condensation of Citral with Methyl-*n*-propylketone, followed by cyclization with Phosphoric acid.

95-169;

## 1275: ETHYL-beta-KETOPELARGONATE

Ethyl heptoyl acetate.

$C_2H_5—OOC—CH_2—CO—(CH_2)_5CH_3$

$C_{11}H_{20}O_3 = 200.28$

Colorless oily liquid. B.P. 252° C.

Almost insoluble in water, soluble in alcohol and oils.

Warm and pleasant, herbaceous-winey, balsamic odor of good tenacity, yet with considerable diffusive power.

This ketoester is rarely offered under its proper chemical name, although it is not a very complicated chemical as such.

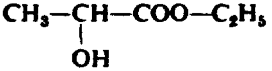
It finds use in perfume compositions for its "mellowing" effect, resembling that of Lavender-Clary Sage undertones, warm notes, versatile herbaceous character, and good tenacity.

Prod.: from Hexyl chloride plus Ethylacetoacetate.

66-874;
see also monograph: Heptyl acetoacetate.

## 1276: ETHYL LACTATE

Ethyl-*alpha*-hydroxypropionate.
Ethyl-*2*-hydroxypropionate.



$CH_3{-}\underset{\displaystyle OH}{\underset{|}{C}}H{-}COO{-}C_2H_5$

$C_5H_{10}O_3 = 118.14$

Colorless liquid, miscible with water, soluble in alcohol and oils. The aqueous solution decomposes slowly. Sp.Gr. 1.04. B.P. 154° C.

Occasionally used as a solvent in perfume compositions. Its mild, ethereal-buttery odor may blend well with certain types of fragrance, but is not always desirable.

Mild, fruity-ethereal, buttery taste in aqueous media. The aqueous solutions become increasingly acid during decomposition of the ester.

Finds quite extensive use in flavor compositions, e.g. in imitation Butter, Butterscotch, Cheese, Coconut, Grape, Maple, Nut, Rum, Strawberry, etc.

Concentrations may vary from 70 ppm in baked goods and 1000 ppm in Brandy, up to 3100 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2440.

4-16; 34-806; 66-786; 100-432; 160-1074; 140-148;

## 1277: ETHYL LAURATE

Ethyl dodecanoate.
Ethyl dodecylate.
Ethyl laurinate.

$CH_3(CH_2)_{10}{-}COO{-}C_2H_5$

$C_{14}H_{28}O_2 = 228.38$

Colorless, slightly oily liquid. Sp.Gr. 0.86. B.P. 269° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Oily-fatty, somewhat leafy and flower-petal-like, mild odor with a trace of a fruity undertone.

Fatty-fruity, not very sweet taste.

Finds very little use in perfumery, except for special creations e.g. floral absolute imitations, where the ester may introduce interesting waxy-oily-green notes, simulating the odor of flower petals, etc. Traces may also be used in artificial Cognac oils for perfumery use.

The ester is used in flavor compositions for imitation Berry, Cheese, Coconut, Cognac, Fruit (complexes), Liqueur flavors, Grape, Nut, Nutmeg, Rum, Spice blends, etc.

Concentration is normally little more than traces, e.g. up to 2 to 17 ppm in the various types of consumer product, except in chewing gum where the concentration may reach 40 ppm.

G.R.A.S. F.E.M.A. No.2441.

Prod.: by direct esterification of Ethanol with Lauric acid under azeotropic conditions.

31-134; 160-1076; B-II-361; 86-18; 4-16; 35-1075; 100-432;

## 1278: ETHYL LEVULINATE

Ethyl laevulate.
Ethyl-*gamma*-ketovalerate.
Acetylpropionic acid, ethylester.

$CH_3{-}CO{-}CH_2{-}CH_2{-}COO{-}C_2H_5$

$C_7H_{12}O_3 = 144.17$

Colorless liquid. Sp.Gr. 1.01. B.P. 206° C.

Soluble in water, miscible in alcohol and oils.

Ethereal-fruity, somewhat green and sweet odor. Mild-fruity, ethereal-green, unripe-Apple-like taste.

This ester is used in flavor compositions, almost exclusively in Apple imitations. It can also be used in Pineapple, Gooseberry, Rhubarb, etc.

The concentration of the ester in the finished consumer product is normally very small, e.g. 6 to 12 ppm.

Prod.: by direct esterification of Ethanol with Laevulinic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2442.

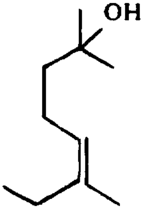
66-881; 160-1078; 100-432;

## 1279: ETHYL LINALOOL

*3*,*7*-Dimethyl-*1*,*6*-nonadien-*3*-ol.

NOTE: The name "Ethyl linalool" is somewhat misleading in that the material is only one Carbon higher homologue than Linalool.

An old name is: Homolinalool.



$C_{11}H_{20}O = 168.28$

Colorless slightly oily liquid. Very slightly soluble in water, soluble in alcohol and oils.

Floral, only slightly woody-green, soft odor of moderate tenacity. The odor type compared to Linalool indicates that "Ethyl linalool" is softer, more waxy, less volatile, less woody-green and overall more floral. It is more Coriander-like, less Bois-de-Rose-like.

This alcohol has been suggested for use in perfume compositions as a modifier for Linalool with certain advantages over that marerial. Ethyl linalool has a somewhat slower rate of evaporation and is easier to work with, needs only normal fixation, and blends with more materials. It introduces softer, more floral-woody, less citrusy notes, according to the composition in which it is used. Along with Ethyl linalyl acetate, it forms a pleasant Bergamot-type background note even in soap perfumes, a combination which is more stable than Bergamot oil itself.

The alcohol is also an interesting item in Muguet, Lilac, Lily, Appleblossom, etc. as well as in fantasy creations.

Prod.: From Methyl ethyl ketone and Acetylene.

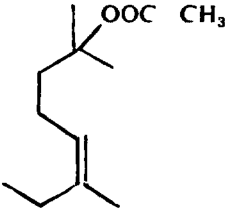
156-234; 96-67;

Sample and data: Hoffmann-laRoche, Inc. Aromatics Div.

## 1280: ETHYL LINALYL ACETATE

*3*,*7*-Dimethyl-*1*,*6*-nonadien-*3*-yl acetate.

Sometimes called: Homo linalylacetate.



$C_{13}H_{22}O_2 = 210.32$

Colorless, slightly oily liquid. Very slightly soluble in water, soluble in alcohol, Propylene glycol, mineral oil and perfume oils.

Sweet, floral, refreshing and rather light odor with a trace of a fruity note. More floral and less fruity than Linalyl acetate.

Sweet, yet slightly woody-floral taste remotely reminiscent of canned pears.

This ester is being used on an increasing scale in perfumery, and seems not only to substitute Linalyl acetate in many cases, but it expands the field of usage of that ester to areas hitherto beyond the effective limits of Linalyl acetate. The subject ester has greater stability, richer odor and better tenacity. It improves the "Bergamot-effect" of a composition where Linalyl acetate has previously been used. It also blends excellently with the conventional perfume and soap perfume materials with almost no limits of application.

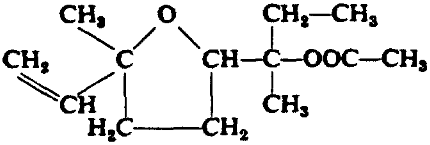
The increased use of Ethyl linalyl acetate is, of course, partly due to the fact that its market price has finally reached the level of its predecessor, Linalyl acetate (1968).

Prod.: by Acetylation of Dehydro-ethyl linalool, followed by hydrogenation of the dehydro-ester.

Sample and data: Hoffmann-laRoche, Inc. Aromatics Div. See also: Ethyl linalool and Ethyl heptenone.

## 1281: ETHYL LINALYL ACETATE EPOXIDE

"Homolinalylacetate epoxide".



$C_{13}H_{22}O_3$ = 226.33

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful and fresh-herbaceous, delicately floral and haylike, warm odor of moderate to good tenacity.

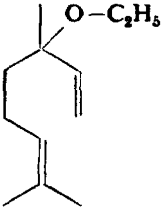
This relatively new ester has been suggested for use in perfume compositions, and is slowly finding its way into many types of fragrance.

Reasonably stable and more powerful than Linalylacetate, it is particularly suitable for soap perfumes, and it offers interesting variations in the Bergamot theme particularly where Bergamot is used along with delicate florals (Muguet, etc.).

(Sample: Hoffmann-laRoche, Inc.).
See also: Linalool oxide.

## 1282: ETHYL LINALYL ETHER

*3*-Ethyl linalool.
Linalyl ethylether.
*3*-Ethoxy-*3*,*7*-dimethyl-*1*,*6*-octadiene.
Do not confuse with Ethyl linalool (see that monograph).



$C_{12}H_{22}O$ = 182.31

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Slightly fruity, primarily sweet-floral odor of moderate to good tenacity. Overall fresher and richer than Linalylacetate, and less green than Methyl linalyl ether.

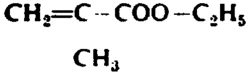
This ether has found some use in perfume compositions, but it has not often been offered under its proper chemical name. It finds use within the companies who have facilities for manufacturing of aroma chemicals.

The recent interest in Ethyl linalool and Ethyl linalylacetate has also increased the interest in other derivatives of Linalool, and the lower alkyl ethers offer pleasant variations with mildly green notes and increased power, very suitable for modern soap and detergent compositions, and for topnotecompositions in finer perfumes.

Prod.: (several methods) e.g. by isomerization of Geraniol in ethylalcoholic environment.

## 1283: ETHYL METHACRYLATE

Ethyl-*alpha*-methyl acrylate.
Ethyl-*iso*-butenoate.
Ethyl-2-methyl-2-propenoate.



$CH_2{=}\underset{CH_3}{C}-COO-C_2H_5$

$C_6H_{10}O_2 = 114.15$

Colorless liquid. B.P. 116° C.

Very slightly soluble in water, soluble in alcohol and oils.

Polymerizes easily in daylight. Commercial material is usually stabilized with Hydroquinone or other inhibitor.

Very diffusive and penetrating, gassy-herbaceous, warm odor of very poor tenacity.

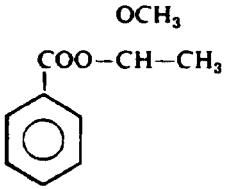
The title material is occasionally used in perfumes where very powerful lift and short "life" is desirable, e. g. in certain types of detergent or automatic dishwashing detergent, in masking compositions for unpleasant, volatile odors, etc.

Prod.: from Acetone via Acetone cyanhydrin to Methyl methacrylate. Ester exchange reaction with Ethanol yields the title ester.

66-635;

## 1284: ETHYL-alpha-METHOXYBENZOATE

*alpha*-Methoxy ethylbenzoate.
*1*-Methoxyethylbenzoate.



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, warm-fruity and woody-spicy odor of moderate tenacity.

Sweet-fruity, slightly spicy taste of Blackcurrant type in concentrations below 20 ppm.

This ester, rarely offered under its proper chemical name, has been suggested for use in flavor compositions of the berry type, mainly Blackcurrant and Cherry.

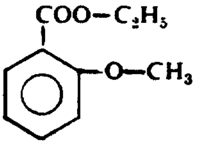
The author is not aware of any use of this material in perfume compositions.

It is not listed in the American Federal Register and not mentioned by the F.E.M.A. wherefore it must not be considered as permissible for food flavors in the U.S.A.

Prod.: (several methods) e.g.: from Vinyl methyl ether and Benzoic acid.

## 1285: ETHYL-ortho-METHOXY BENZOATE

"Ethyl salicylate, methyl ether".
"Ethyl methyl salicylate" (misleading name).
Ethyl-*ortho*-anisate.



$C_{10}H_{12}O_3 = 180.21$

Colorless, slightly viscous liquid. B.P. approximately 254° C. Sp.Gr. 1.11.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Sweet, floral, heavy-fruity, warm odor of good tenacity. The floral notes resemble Hyacinth, Wistaria and Ylang-Ylang, while the fruity notes have a delightful complex of Grape, Orange and Wintergreen sweetness.

Powerful, sweet fruity taste, reminiscent of Concord Grape with distinct notes of Wintergreen.

This ether-ester is used in perfumery for its heavy-floral and warm effects in Hyacinth, Cananga, Ylang-Ylang, Orange blossom, Wistaria and many other floral complexes. It creates interesting complexes with Coumarin derivatives.

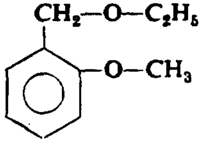
Although not listed specifically in the U.S. Federal Register as G.R.A.S., this material could become an interesting flavor item, once it is approved for food use. It introduces warm sweetness in Grape flavor compositions, depth in Prune and Plum, Raisin, Rum etc., and could find a place in many types of flavor formulations.

Prod.: by Methylation of Ethyl salicylate.

7-209; 8-137;
See also: *ortho*-Methoxy methylbenzoate.

## 1286: ETHYL-ortho-METHOXY BENZYLETHER

*ortho*-Methoxy benzyl ethyl ether.



$C_{10}H_{14}O_2 = 166.22$

Colorless, slightly oily liquid. Insoluble in water, soluble in alcohol and perfume oils.

Very powerful and diffusive, warm-floral, pungent odor, reminiscent of Hyacinth at high concentration, of Rose at proper dilution.

This ether has found much use in floral bases on account of its power and excellent stability in soap. Its ability to make the conventional Rose materials smell more "rosy" and Hyacinth-materials smell more "Hyacinth-like", are just a few of the many possible applications. The use level will often be less than one percent in a perfume oil, but may be much higher in special bases.

It is interesting to note the relationship between this ether and the naturally occurring Methyl phenylethyl ether (in Pandanus or "Kewda"-oil), and it is obvious that the development of the subject ether and related ethers have come out of the study of the Kewda oil.

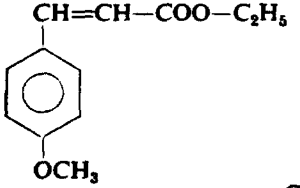
Prod.: from *ortho*-Anisaldehyde (methylated Salicylic aldehyde) by hydrogenation, followed by reduction with Sodium methylate and Ethylation with Ethyl sulfuryl ether in a non-ionic solvent.

Other methods start with Salicylic aldehyde, and the Methylation may be undertaken with Dimethyl sulfate, reduction by various means, the Ethylation with Diethyl sulfate.

See also: Ethyl phenylethyl ether, and: Methyl phenylethyl ether, and: 104-504;

## 1287: ETHYL-para-METHOXY CINNAMATE

*4*-Methoxy ethylcinnamate.



$C_{12}H_{14}O_3 = 206.24$

White crystals. Insoluble in water, soluble in alcohol and oils.

Very faint, sweet-balsamic-anisic odor of good tenacity.

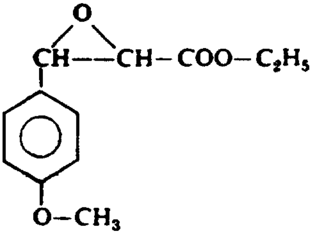
This ether-ester is comparatively rare and has apparently very little significance in perfumery.

It has been suggested for use in floral and balsamic-Oriental compositions, but it does not seem to offer any unusual or irreplaceable notes. Most perfume laboratories do not have and have never had this item on their shelf.

Prod.: by esterification of Ethanol with the Methylether of *para*-Coumaric acid.

## 1288: ETHYL-beta-para-METHOXY-PHENYL GLYCIDATE

**Ethyl anisyl glycidate.**
*para*-Methoxyphenylglycidic acid, ethylester.
*alpha-beta*-Epoxy-*beta*(*para*-Methoxyphenyl) propionate.



$C_{12}H_{14}O_4 = 222.24$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous odor reminiscent of sweet, semi-dried hay. Only mildly fruity notes are perceptible, the sweetness being more floral-ethereal than fruity, when the material is compared to the Ethyl methyl phenyl glycidate.

This glycidic ester has been suggested for use in perfume compositions of the herbaceous or herbaceous-floral character, supporting Amylsalicylate, Lavender-Lavandin, Clary Sage, Terpineol, etc. It blends excellently with Anisaldehyde in Lilac or Fougères.

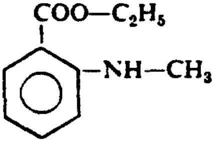
The author is not aware of any significant use of this ester in flavor compositions.

Prod.: from Anisaldehyde plus Ethylmonochloroacetate and Sodium methylate.

3-206;

## 1289: ETHYL-N-METHYL ANTHRANILATE

*N*-Methylanthranilic acid, ethylester.



$C_{10}H_{13}NO_2 = 179.22$

Colorless or pale straw-colored liquid.
Sp.Gr. 1.12. B.P. 278° C.

Almost insoluble in water, soluble in alcohol and perfume oils, poorly soluble in Propylene glycol.

Sweet and soft fruity-floral odor, reminiscent of Petitgrain or Mandarin-petitgrain oils. Excellent tenacity.

Grape-like (Concord type), winey and sweet taste of considerable power.

This ester has found a little use in perfume compositions as a variant of the conventional "Orangeblossom"-type of Anthranilates. It blends excellently with the Citrus oils, in Fougère themes, in Lavender fantasy compositions, in Magnolia and Honeysuckle and many other heavy floral bases. It has very little tendency to form strong-colored condensation products with aldehydes, except for the fact that most "Di-anthranilates" contain a significant proportion of the Mono-ester, which causes strong coloration with aldehydes.

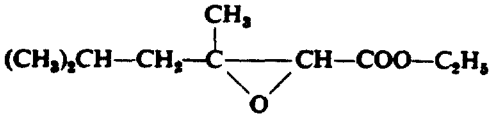
The ester could find use in flavor compositions, not only for Grape and Mandarin, but for many types of fruit, and in the popular "Tutti-frutti" theme. Its great power and tenacity gives it advantages for use in hot-processed candy or other food products.

Prod.: from *N*-Methylanthranilic acid and Ethyl alcohol, by azeotropic type esterification, or:
by Methylation of Ethyl anthranilate with Dimethyl sulfate.

34-1012; 86-19; 4-17;

## 1290: ETHYL METHYL-iso-BUTYLGLYCIDATE

Ethyl-*2,3*-epoxy-*3,6*-dimethylhexanoate.



$C_{10}H_{18}O_3 = 186.25$

Colorless or very pale straw-colored liquid.

Almost insoluble in water, soluble in alcohol and oils. Slightly soluble in Propyleneglycol.

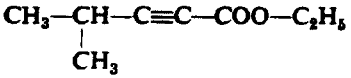
Sweet and warm, rich-fruity odor with caramellic undertone. The fruity notes are rather uncharacteristic, but have some resemblance to Strawberry-Pineapple. There is also some resemblance to the odor of Ethyl phenyl glycidate.

This glycidate has been manufactured as a member of a long line of homologues in search of new and interesting fruity odorants. However, the author finds that it is not one of the more useful members of this family, and it is most likely that the subject material will remain in the research chemical collection and never reach the commercial pricelists.

Prod.: from Methyl-*iso*-butylketone via Darzen-Claisen reaction.

## 1291: ETHYL-3-METHYL-n-BUT-1-YNE CARBONATE

Ethyl-*iso*-hexynoate.



$$CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-C\equiv C-COO-C_2H_5$$

$C_8H_{12}O_2 = 140.18$

Colorless mobile liquid. B.P. 183° C.

Almost insoluble in water, soluble in alcohol and oils, very poorly soluble in Propylene glycol.

Powerful and diffusive, foliage-green odor, practically without trace of fatty or "greasy" notes. However, the initial impression is that of a rather unnatural green, although it could be classified as a "Lilac-green" type of odor.

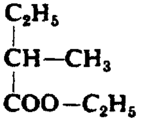
This acetylenic ester is rarely offered commercially under its proper name, but it occurs in a few specialties as part of the green theme. The main drawback of this material is its volatility, demanding a very solid fixation in order to produce a pleasant level of slowly released green notes. It offers interesting notes as a modifier in a complex of green odors, and blends very well with Oakmoss and Citrus oils. In view of the commercial production of an almost complete line of Hexenyl esters, etc., it is most conceivable that the acetylenic esters will slowly become obsolete, generally considered more irritating to the skin than the olefinic derivatives.

Prod.: from *iso*-Valeric aldehyde via *3*-Methylbut-*1*-yne to the acid, from which subject ester is produced by conventional method.

5-245;

## 1292: ETHYL-2-METHYLBUTYRATE

Methyl ethyl acetic acid, ethylester.



$$\begin{array}{l} C_2H_5 \\ | \\ CH-CH_3 \\ | \\ COO-C_2H_5 \end{array}$$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. Very slightly soluble in water, soluble in alcohol and Propylene glycol, miscible with perfume and flavor oils.

Powerful and diffusive, green-fruity, pungent odor, reminiscent of Apple peels, Pineapple skins or the peels of unripe plums.

The subject ester has found some use in fruit flavor compositions at very low concentration – equivalent to about 0.5 to 5 ppm in the finished product.

The parent acid and the corresponding alcohol and many of its esters have been identified in natural food products and essential oils. New perfume and flavor materials have subsequently been produced and marketed.

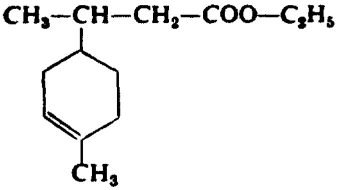
Prod.: by esterification of Ethyl alcohol with Methyl ethyl acetic acid.

G.R.A.S. F.E.M.A. No.2443.

B-II-304; The Glidden Co., 1967.

## 1293: ETHYL-beta-(4-METHYL-3-CYCLOHEXENYL)-BUTYRATE

Ethyl-*beta-para*-dimethyl tetrahydrophenylpropionate (*1,2,3,6*).



$C_{13}H_{24}O_2$ = 212.34

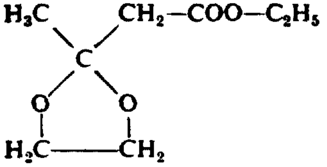
This rare ester has been used in perfumery for its warm-spicy, moderately tenacious odor, often compared to that of Nutmeg. It is true that it does carry some of the characteristics of Nutmeg oil odor, but this is a very complex odor and needs more than one chemical to demonstrate similarity.

The title ester was covered by U.S. patent No. 2.556.150 of 26th Dec. 1946, and since the material has not been freely marketed, there is reason to believe that it has failed to interest the perfumers.

The ester is briefly mentioned in this work as an example of an unusual type of perfume ester.

## 1294: ETHYL-2-METHYL-1,3-DIOXOLANE-2-ACETATE

Fructone (I.F.F.).



$C_8H_{14}O_4$ = 174.20

Colorless or pale straw-colored, slightly viscous liquid. Very slightly soluble in water, soluble in alcohol and Propylene glycol, miscible with most perfume oils.

This cyclic ketal has found some use in perfumery due to its pleasant warm-fruity, winey and sweet odor.

The material introduces natural notes in many types of warm-floral bases, Jasmin, Peony, Gardenia, Sweet Pea etc., and its fruity-winey character blends well with Labdanum in many non-floral fragrance types.

In spite of its pleasant "fruit-preserve" taste, this material is – to the author's knowledge – not used in flavor compositions.

Prod.: by condensation of Ethyl acetoacetate with Ethylene glycol in presence of a catalyst and under conditions of azeotropic distillation to remove water formed under condensation.

See also: Ethyl-*2,4*-dimethyl-*1,3*-dioxolane-*2*-acetate.

## 1295: ETHYL-6-METHYL-n-HEPT-5-EN-1-YNE CARBONATE

Ethyl-*iso*-nonenynoate.

$(CH_3)_2C{=}CH{-}CH_2{-}CH_2{-}C{\equiv}C{-}COO{-}C_2H_5$

$C_{11}H_{16}O_2$ = 180.25

Colorless mobile liquid. B.P. 240° C.

Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Powerful leafy-green, but rather gassy-pungent odor of moderate to good tenacity.

In extreme dilution the odor is more agreeable, but still not very natural.

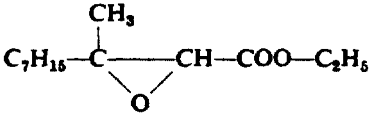
This acetylenic ester has been used in perfume compositions for its powerful green effect, but the author believes that the material has become obsolete in competition with more natural smelling acetylenic esters and lately, in competition with the Hexenols and esters.

Prod.: from Methylheptenone via *6*-Methyl-*n*-hept-*5*-en-*1*-yne to the acid from which the ester is prepared.

5-245;

## 1296: ETHYL METHYL HEPTYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3*-methyl decanoate.



$C_{13}H_{24}O_3 = 228.34$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, non-descript fruity odor of moderate tenacity. Sweet, fruity taste of Raspberry-Peach-like type.

This glycidic ester has been suggested for use in flavor compositions as a modifier for the more common glycidates. It is less powerful than the Ethyl methylphenyl glycidate, but it is also milder in its sweetness, obviously free from any trace of Acetophenone-like harshness, a common drawback of commercial grade EPMG.

The title material is rarely offered commercially, and it may well become obsolete since it does not offer any unusual or highly interesting effects in flavor creations.

The use in perfume compositions is negligible.

Prod.: from Methylheptylketone (*2*-Nonanone) via glycidic ester synthesis.

See also: 3-167;

## 1297: ETHYL-6-METHYL-n-HEPT-1-YNE CARBONATE

Ethyl-*iso*-nonynoate.
Ethyl-*6*-methyl-*2*-octynoate.
Ethyl methyl heptincarbonate.

$$(CH_3)_2CH—CH_2—CH_2—CH_2—C\equiv C—COO—C_2H_5$$

$C_{11}H_{18}O_2 = 182.27$

Colorless mobile liquid. B.P. 226° C.

Insoluble in water, soluble in alcohol and oils. Almost insoluble in Propylene glycol.

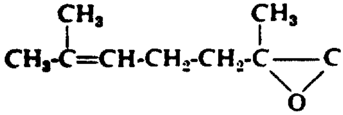
This ester, as such, has very little importance in perfumery. It has occurred as component in perfume specialties and bases, offering a powerful green foliage type odor. It is less "gassy" than the conventional acetylenic esters, but since the material is not offered as a pure, single chemical, there has been little interest in it. Recent availability of a wealth of Hexenyl esters covering almost every nuance of the natural green odor has also made the title material obsolete.

Prod.: from Methyl-*iso*-hexylketone via 6-Methyl-*n*-hept-*1*-yne to the acid from which the Ethylester is prepared.

5-245;

## 1298: ETHYL METHYL-iso-HEXENYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3,7*-dimethyl-*6*-octenoate.
*iso*-Hexenylmethylglycidic acid, ethylester.



$$\mathrm{CH_3\text{-}\overset{\overset{CH_3}{|}}{C}=CH\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{CH_3}{|}}{C}\underset{\diagdown\,O\,\diagup}{——}CH\text{-}COO\text{-}C_2H_5}$$

$C_{12}H_{20}O_3 = 212.29$

Colorless or pale straw-colored, oily liquid. B.P. 242° C. Sp.Gr. 0.99.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Mild and sweet-fruity, slightly green, caramellic-vegetable type odor of moderate to good tenacity. Often compared to the odor of Quince.

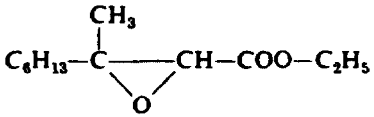
Although very few materials of "Quince" type are available to the perfumer or flavorist, this glycidic ester has not found much use in perfumes or flavors. It is mild (which is appropiate for a Quince type) but it lacks character for the perfumer and power for the flavorist. Some of the lower homologues or relatives of this ester have found more extensive use.

Prod.: from Methylheptenone plus Ethyl monochloroacetate plus Sodium methylate.

Riechstoffe und Aromen, August 1956, page 234.
See also: Methyl-*3,5*-dimethyl-*2,3*-epoxy-*4*-hexenoate.

## 1299: ETHYL METHYL HEXYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3*-methylnonanoate.
(Do not confuse with Ethyl-*iso*-hexenyl methylglycidate).



$$\mathrm{C_6H_{13}—\overset{\overset{CH_3}{|}}{C}\underset{\diagdown\,O\,\diagup}{———}CH—COO—C_2H_5}$$

$C_{12}H_{22}O_3 = 214.31$

Colorless liquid. Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet, Strawberry-Raspberry-Pear-like odor of moderate tenacity.

Fruity-caramellic, Strawberry-Pear-like taste in concentrations below 50 ppm.

This glycidic ester has been suggested for use in perfume compositions as a modifier for the conventional glycidic esters, e.g. in lipstick perfumes and other fragrance types calling for mild-fruity notes.

It is not listed in the American Federal Register or mentioned in the G.R.A.S. list of F.E.M.A. Accordingly, it should be considered as banned from use in flavor compositions in the U.S.A.

Prod.: from Methyl-*n*-hexyl ketone with Ethyl monochloroacetate and Sodium methylate catalyst.

See also: Ethyl-*iso*-hexenyl methyl glycidate and Methyl-*3,5*-dimethyl-*2,3*-epoxy-*4*-hexenoate.

## 1300: ETHYL-5-METHYL-n-HEX-1-YNE CARBONATE

Ethyl methyl hexin carbonate.
Ethyl-*iso*-octynoate.

$(CH_3)_2CH—CH_2—CH_2—C{\equiv}C—COO—C_2H_5$

$C_{10}H_{16}O_2 = 168.22$

Colorless liquid. B.P. 212° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Powerful and very diffusive, fresh-green, oily but not waxy odor of poor tenacity.

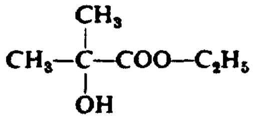
This acetylenic ester has, like most of its homologues, outlived its days in perfumery and may well be considered as obsolete or almost obsolete. The possibility of these materials being highly skin-irritating, and the appearance of less hazardous, more natural smelling Hexenyl esters at similar cost has contributed to the gradual disappearance of all these odd acetylenic esters from the perfume chemicals price lists.

Prod.: from Methyl ethyl ketone via *5*-Methyl-*n*-hex-*1*-yne to the acid from which the Ethylester is prepared.

5-245;

## 1301: ETHYL METHYL LACTATE

*alpha*-Methyl-*alpha*-hydroxypropionic acid, ethylester.



$$CH_3-\overset{\overset{CH_3}{|}}{\underset{\underset{OH}{|}}{C}}-COO-C_2H_5$$

$C_6H_{12}O_3 = 132.16$

Colorless liquid. Somewhat soluble in water, miscible with alcohol, soluble in most oils.

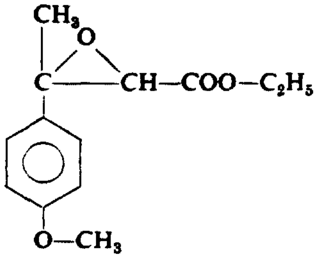
Refreshing, herbal-green, vinous odor with a faint resemblance to garden Mint or Spearmint.

Although mentioned in perfumery literature, this ester has – to the author's knowledge – little, if any, application in perfume or flavor compositions. It is quite possible, however, that the esters of ethylated or methylated Lactic acid have odors of some interest, and that a certain amount of confusion in nomenclature exists.

31-134;
See also: Ethyl ethyl lactate.
Ethyl-*alpha*-ethoxypropionate: see 66-789;
Methyl-*alpha*-ethoxypropionate: see 66-789;

## 1302: ETHYL-beta-METHYL-beta-para-METHOXYPENYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3*-methyl-*3*-(*para*-methoxyphenyl)-propionate.
Ethyl methyl anisyl glycidate.



$C_{13}H_{16}O_4 = 236.27$

Colorless oily liquid.

Sweet-herbaceous, anisic type odor of good tenacity and with only very mildly fruity undertones.

Anisic-Raspberry-like taste in concentrations lower than 20 ppm. A slightly bitter note seems to accompany the taste at all concentrations above the minimum perceptible.

This glycidic ester has been suggested for application in perfume compositions as a modifier for the conventional esters in Lilac, Magnolia, Appleblossom and other mild, sweet-floral types. It blends well with Heliotropine, Anisaldehyde, Terpineol and Phenylethylalcohol, and it creates pleasant nuances with Undecanolide or with the Ionones.

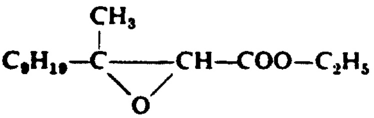
It is rarely offered commercially under its proper chemical name, and it does not rate among the most popular glycidic esters.

Prod.: from *para*-Methoxy acetophenone (Acetanisole) with Ethylmonochloroacetate and Sodium methylate.

3-286;

## 1303: ETHYL METHYL NONYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3*-methyl dodecanoate.



$C_{15}H_{28}O_3 = 256.39$

Colorless or very pale straw-colored oily liquid. B.P. 271° C. Sp.Gr. 0.93.

Almost insoluble in water, soluble in alcohol and oils, fairly soluble in Propylene glycol.

Pleasant Banana-Raspberry-type odor.

Moderate tenacity.

Sweet fruity taste of Banana-Raspberry-Mango type.

This glycidic ester has found some use in perfumery where it may introduce pleasant variations in the conventional Ethylmethylphenylglycidate theme in fruity lipstick fragrances, etc.

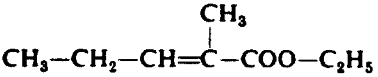
The ester is used in flavor compositions outside of the U.S.A., where it is not listed specifically as G.R.A.S. It is by many flavorists considered superior as a Raspberry chemical when compared to Ethylmethylphenylglycidate.

Prod.: from Methyl nonyl ketone with Ethyl monochloroacetate and Sodium methylate catalyst.

77-197; see also: Riechstoffe und Aromen, August 1956, page 234.

## 1304: ETHYL-2-METHYL-2-PENTENOATE

2-Methylpentenoic acid, Ethylester.



$$CH_3-CH_2-CH=\overset{\overset{CH_3}{|}}{C}-COO-C_2H_5$$

$C_8H_{14}O_2 = 142.20$

Colorless mobile liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful, fruity-green, diffusive odor of Banana-Pineapple type, in proper dilution also reminiscent of Strawberry.

Sweet fruity Strawberry-Banana like taste. Pleasant taste level is about 10 ppm or lower.

This ester, although comparatively simple, is rarely offered under its proper chemical name. It is manufactured by a number of creative flavor or perfume houses for "captive" use in fragrances and – mostly – in flavor compositions.

The alcohol, corresponding to the parent acid is Methylpentenol, which is relatively well known in perfumery as a "green" odorant.

The title ester is not mentioned in the United States Federal Register or listed by F.E.M.A. as G.R.A.S. wherefore it should be considered as banned from use in food flavors in the U.S.A.

Prod.: by esterification of 2-Methyl-2-pentenoic acid with Ethanol.

## 1305: ETHYL-4-METHYL-n-PENT-1-YNE CARBONATE

Ethyl-*iso*-heptynoate.

$$(CH_3)_2CH-CH_2-C{\equiv}C-COO-C_2H_5$$

$C_9H_{14}O_2 = 154.21$

Colorless liquid. B.P. 211° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

The subject acetylenic ester is one of very little interest to the perfumer, but the material is included in this work for the sake of completing the description of most of the acetylenic esters which have at one time or another been commercially available or have been of some interest to the creative perfumer.

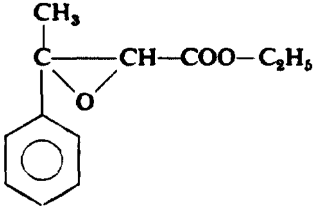
The title material has a powerful, but rather sharp green odor of very poor tenacity. It is less stable than Methylheptin carbonate but its odor is considered slightly superior to that of MHC in that it is less fatty. It is possible that the manufacture of the title ester includes problems other than the common ones, and the cost is therefore prohibitive for its wider use.

Prod.: from Methyl-*iso*-butylketone via *4*-Methyl-*n*-pent-*1*-yne to the acid from which the Ethylester is prepared.

5-245;

## 1306: ETHYL METHYL PHENYL GLYCIDATE

Methylphenyl glycidic acid, ethylester.
"Strawberry aldehyde".
"Aldehyde C-16" (so-called).
"Fraise".
"Fraiseol".
Ethyl-*3*-methyl-*3*-phenylglycidate.
Ethyl-*alpha-beta*-epoxy-*beta*-methylphenyl-propionate.
E.M.P.G.



$C_{12}H_{14}O_3 = 206.23$

Colorless, slightly viscous liquid. B.P. 260°C. Sp.Gr. 1.10.

Almost insoluble in water, poorly soluble in Propylene glycol, Glycerin and mineral oil, soluble in alcohol, miscible with most perfume and flavor oils.

Sweet-fruity, "candy"-like, warm odor with considerable similarity to that of Strawberry juice or Strawberry syrup.

Sweet and distinctly fruity taste with good resemblance to Strawberry and also other berry-type of fruit. Concentrations in aqueous media higher than 50 ppm tend to give harsh, pungent or burning effect unless the material is accompanied by suitable sweeteners and modifiers in a flavor composition.

NOTE: The ester may yield Hydratropic aldehyde as a result of hydrolysis.

This ester is used in perfume compositions not only for its fruity note which is utilized in lipstick perfumes with Ionones and fruity Lactones, but also as a sweetener in floral complexes for use in fragrance types other than the typical floral ones, e.g. Chypre, Oriental, etc. It blends well with the aliphatic aldehydes for sweet and powerful topnote base complexes, with Hydroxycitronellal, Ionones, Nonanolide and Undecanolide, etc. in floral or sweet-woody or woody-aldehydic bases, and it is a classical item in Rose compositions.

It is widely used in flavor compositions, not only Strawberry imitation, but also other berry flavors, Raspberry, Gooseberry, in Banana variations, Cherry, Grape, Pineapple, Coconut ,Liqueur, Wine, Tutti-frutti, "juicy-fruit" and other fantasy flavors.

Concentrations vary from 5 to 20 ppm in candy up to 450 or 500 ppm in chewing gum.

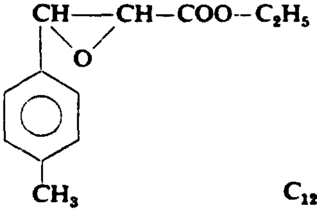
Prod.: from Acetophenone by condensation with Ethyl monochloroacetate in alkaline solution, using Sodamide as condensing agent.

G.R.A.S. F.E.M.A. No.2444.

4-95; 5-272; 31-50; 77-197; 68-926; 86-3; 86-19; 106-42; 157-84; 140-152;

## 1307: ETHYL-para-METHYL-beta-PHENYL GLYCIDATE

Ethyl-*para*-tolyl glycidate.
"Raspberry aldehyde" (so-called).
"Aldehyde C-20" (so-called).
Ethyl-*para*-M.P.G.
Ethyl-*alpha-beta*-epoxy-*beta* (*para*-methyl-phenyl)-propionate.
"Aldehyde C-17" (sometimes called).



$C_{12}H_{14}O_3 = 206.23$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol, miscible with most perfume and flavor materials. Poorly soluble in Propylene glycol and mineral oil, almost insoluble in Glycerin.

Distinctly fruity, but also somewhat woody odor, less sweet (more dry) than the Ethyl methyl phenyl glycidate.

Fruity, rather nondescript taste, unless incorporated in a complex with other flavor materials; quite powerful.

This ester is almost exclusively used in perfumery. It offers an interesting variation from the E.M.P.G. (regular) in that it may create Raspberry notes in combination with Ionones and other aromatics. It gives interesting effects with woody materials, Vetiver, Orris and the Cyclohexyl derivatives. Such combinations may serve as basis for Chypre or Oriental bases, etc.

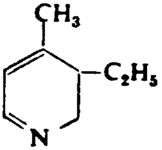
Although not listed as G.R.A.S. by the U.S. Federal Register, this ester is probably used in other countries for its Raspberry effect in flavor compositions, and as a modification of the conventional E.M.P.G.

Prod.: by condensation of *para*-Methylbenzaldehyde with Ethyl monochloroacetate in alkaline solution, using Sodamide as condensing agent.

86-3; 140-152;

## 1308: 3-ETHYL-4-METHYL PYRIDINE

*4*-Methyl-*3*-ethyl pyridine.



$C_8H_{11}N = 121.18$

Almost colorless or very pale amber-colored oily liquid.

Slightly soluble in water, soluble in alcohol and oils.

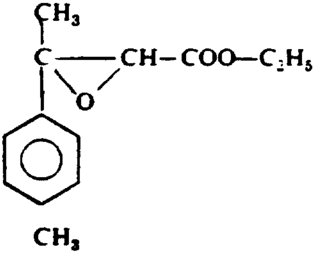
Sweet-woody, herbaceous and slightly spicy-earthy odor of moderate tenacity.

This alkyl-substituted Pyridine has been suggested for use in perfume compositions of the non-floral character. It blends excellently with Oakmoss and Vetiver, the earthy-mossy notes of which it will support and modify in a pleasant manner, and it produces new shades of Fougère with Amylsalicylate, Cedarwood, Lavender, Amylvinylcarbinol etc.

Sample: Reilly Tar and Chemical Corp., Indianapolis, U.S.A.

## 1309: ETHYL METHYL-para-TOLYL GLYCIDATE

Ethyl methyl-*para*-methyl phenyl glycidate.
E.M.-*para*-M.P.G.
Ethyl-*alpha-beta*-epoxy-*alpha*-methyl-*beta*-(*para*-methylphenyl)-propionate.



$C_{13}H_{16}O_3 = 220.24$

Colorless or pale straw-colored, viscous liquid.

Insoluble in water, soluble in alcohol and most perfume and flavor materials.

Mild, deep-fruity, slightly floral and woody odor with "cooked fruit" undertones and very great tenacity.

Fruity, but not distinctly sweet taste. Somewhat dry undertone.

This ester, which is comparatively rare, finds a little use in perfume compositions for its lasting, fruity character, and for its ability to blend and create pleasant blends with the Ionones, Cedarwood derivatives, Butylcyclohexanyl acetate and many other woody or Orris-like materials. It has less tendency to produce harsh topnotes than e.g. Ethyl methyl phenyl glycidate, but it does not offer any very natural fruit notes, unless accompanied by the conventional materials for such notes. It has good fixative properties for the volatile fruit esters and may round off the rough or harsh topnotes of many perfume chemicals.

The author is not aware of its use in flavor compositions.

Prod.: from *para*-Methyl acetophenone and Ethyl monochloro acetate by condensation, using Sodamide as condensing agent in alkaline solution.

## 1310: ETHYL MYRISTATE

Ethyl tetradecanoate.

$CH_3(CH_2)_{12}COO—C_2H_5$

$C_{16}H_{32}O_2 = 256.43$

Colorless oily liquid, solidifying in the cold. M.P. 12° C. B.P. 295° C. Sp.Gr. (liquid) 0.86.

Insoluble in water, soluble in alcohol and perfume and flavor materials.

Very mild oily-ethereal odor with some resemblance to Orris and Violet.

Finds some use in perfume compositions as a modifier/blender in floral complexes, artificial flower absolutes (Tuberose-Gardenia etc.) and in Ionone-Orris complexes.

Used in flavor compositions for imitation Coconut, Honey, Cognac, Quince and in fruit complexes.

Concentration in Liqueurs would be about 6 to 30 ppm.

G.R.A.S. F.E.M.A. No.2445.

Prod.: by direct esterification of Ethanol with Myristic acid, using azeotropic conditions.

31-134; 35-1075; 61-85; 77-188; 28-608; 4-17; 100-433;

## 1311: ETHYL NITRATE and ETHYL NITRITE

"Ethyl nitrate spirits".
Nitric ether, alcoholic solution.
"Spirit of nitrous ether".
Nitrous and Nitric ethers, alcoholic solution.

Nitrous ether: $C_2H_5—O—NO = 75.07$
Nitric ether: $C_2H_5—O—NO_2 = 91.07$

The commercial product is a colorless mobile liquid, boiling range 57 to 78° C. Sp.Gr. 0.81.

Soluble in water, alcohol and oils.

Very diffusive, sweet, ethereal odor. Sweet "fermented-fruit"-like taste. Nitrous ether is a gas at room temperature, B.P. 17° C. Sp.Gr. 0.90.

Prod.:

1) from Ethyl alcohol in 10% aqueous solution plus Nitrosyl chloride.
2) from Sodium Nitrite plus Ethyl alcohol with Sulfuric acid in the cold.

Nitric ether is a volatile liquid. B.P. 88° C. Sp.Gr. 1.10 and slightly soluble in water.

The commercial product and the Nitrous ether in particular are highly flammable and the vapors form explosive mixtures with air.

Used in flavor compositions for imitation Arak, Cherry, Brandy, Strawberry, Pineapple, Liqueur, Rum, etc.

Concentration is normally mere traces, e.g. 0.1 to 10 ppm but may reach 50 ppm in certain types of syrup.

G.R.A.S. F.E.M.A. No.2446.

4-17; 86-19; 100-433; B-I-329; 26-546; 66-335; 66-336;

## 1312: ETHYL NONANOATE

Ethyl pelargonate.
Ethyl nonylate.
Pelargonic ether (old name).

$CH_3(CH_2)_7\text{—}COO\text{—}C_2H_5$

$C_{11}H_{22}O_2 = 186.30$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 228° C.

Insoluble in water, soluble in alcohol, Propylene glycol and oils.

Slightly fatty-oily, fruity and nut-like odor with a winey undertone. Fatty-nutty and delicately fruity, Apricot-type taste with a trace of a rosy note.

This ester is used in perfume compositions in very discrete amounts to introduce natural floral-fruity character, mainly in topnotes for Rose and Citrus type fragrances, but also in general to support power and freshness in topnotes.

It is widely used in flavor compositions for imitation Apple, Apricot, Quince, Cognac, Coffee, Grape, Pear, Quince, Wine, as well as in numerous berry types, partly as a modifier for Ethyl heptoate.

The nut-like note, characteristic of many C-9 derivatives, is utilized in Coconut, Hazelnut, etc.

Concentrations are about 4 to 40 ppm in icings and other sugar-rich products, but may run as high as 500 to 600 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2447.

Prod.: by direct esterification of Ethanol with Nonanoic acid under azeotropic conditions.

4-17; 26-548; 35-514; 43-501; 7-172; 86-19; 77-187; 106-151; 103-91; 158-186; B-VI-470; 140-142;

## 1313: ETHYL NONIN CARBONATE

Ethyl nonyne carboxylate.
Ethyl decynoate.
Ethyl-*2*-decynoate.

$CH_3(CH_2)_6C{\equiv}C\text{—}COO\text{—}C_2H_5$

$C_{12}H_{20}O_2 = 196.29$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Sweet-green and slightly waxy odor, nearest in type to Methyl decin carbonate. Sweeter and more waxy than Methyl octin carbonate.

Although this ester has been available at times, it remains a very rare item, but it is not missed by the perfumers. The tendency toward new green odorous chemicals is not in favor of the Acetylenic esters, few of which can truly be classified as "natural green" odors.

The title material is mentioned mainly for the sake of completing the description of the Acetylenic esters.

Prod.: from Methyl-*n*-heptyl ketone via Nonyne and its acid to the ester.

## 1314: ETHYL NONYLENATE

Ethyl-*2*-nonenoate.
"Homo-neofolione".

$CH_3(CH_2)_5CH\text{=}CH\text{—}COO\text{—}C_2H_5$

$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid. Very slightly soluble in water, soluble in alcohol, miscible with perfume oils.

Herbaceous-green, leafy, Violet-leaf type odor with Coconut-like undertones.

The herbaceous notes are more pronounced that in the Methylester (Neofolione, Givaudan), and the Coconut-like notes somewhat more suppressed.

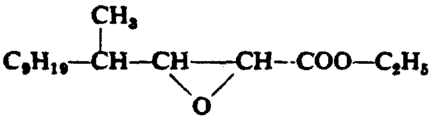
This ester, not nearly as well-known as the Methylester, finds a little use in perfumery as a modifier for its lower homologue, or as a variation from the conventional Violet-leaf theme. The delicate fatty-nut-like notes blend well with Ionones or floral complexes in Lily, Narcissus, etc.

Prod.: by direct esterification of Ethanol with Nonenoic acid which is commercially available. Azeotropic conditions.

4-17;

## 1315: ETHYL NONYL ETHYL GLYCIDATE

Ethyl-*2,3*-epoxy-*4*-methyl tridecanoate.



$C_{16}H_{30}O_3 = 270.42$

Colorless or very pale straw-colored viscous liquid. B.P. 289° C. Sp.Gr. 0.93.

Almost insoluble in water, soluble in alcohol and oils. Slightly soluble in Propylene glycol.

Fresh-fruity, sweet Lemon-like citrusy odor of good tenacity.

Sweet-fruity, refreshingly Lemon-like taste (type: terpeneless Lemon) at concentrations below 30 ppm.

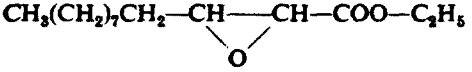
This glycidic ester – very rarely offered commercially under its proper chemical name – has found some use in flavor compositions as a fixative-blender in Citrus flavors, particularly Lemon, but also in Peach, Apricot, Mango, etc.

It is not listed by the United States Federal Register or mentioned in any G.R.A.S. list by F.E.M.A. and should therefore be considered as banned from use in food flavors in the U.S.A.

Prod.: from Methyl nonyl acetaldehyde with Ethyl monochloroacetate and Sodium methylate catalyst.

## 1316: ETHYL NONYL GLYCIDATE

Ethyl-*2,3*-epoxy dodecanoate.



$C_{14}H_{26}O_3 = 242.32$

Colorless oily liquid. B.P. 276° C.
Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils, fairly soluble in Propylene glycol.

Sweet, mild, Orange-peel-like odor of moderate tenacity.

Sweet citrusy taste, but not very powerful.

The title ester, only occasionally offered commercially, has been recommended for use in perfumes and flavors, but does not seem to have gained much popularity. It may be a component of certain specialties, but is rarely found on the shelf in a perfume or flavor laboratory.

It is interesting, however, to notice the odor/flavor type of this epoxydodecanoate with the recent findings of new components in Orange peel in mind (Dodecadienal, Dodecenal, etc.). The unsaturated aldehydes are, of course, much more powerful and natural, and are finding increased use in perfumes and flavors. The interest in glycidic esters seems to have dwindled except for a few items, whatever the reason for this lack of interest may be.

Prod.: from Decanal ("Aldehyde C-10") with Ethyl monochloro acetate and Sodium methylate.

Lit: Riechstoffe und Aromen, August 1956, page 234.

## 1317: ETHYL OCTIN CARBONATE

Ethyl-*2*-nonynoate.
Ethyl octyne carboxylate.
This ester is often marketed in mixtures with other acetylene carboxylic esters.

$CH_3(CH_2)_5C{\equiv}C{-}COO{-}C_2H_5$

$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. B.P. 221° C. Sp.Gr. 0.93.

Insoluble in water, soluble in alcohol and oils, slightly soluble in Propylene glycol.

Delicate, yet intensely Violet-leaf-like, green odor, also reminiscent of vegetables, Cucumber, etc.

Its overall performance shows softer notes than those of the Methylester, in fact it is probably the mildest smelling of all the commonly used Acetylenic acid esters.

This ester finds some use in perfume compositions, mainly in the creation of fresh topnotes and as a foliage note in certain types of Rose fragrance. It blends well with the Ionones, although it is generally agreed (according to the author's impressions) that the Acetylenic acid esters are on their way out of perfumery, being replaced with more natural-smelling, easier-to-incorporate, and stabler perfume chemicals, particularly those of the Hexenol series, and the Nonadienol-family.

The subject ester is used in flavor compositions to introduce a green or "unripe-fresh" note in Berry imitations, Melon flavors and various fruit complexes.

The concentration used is normally about 0.5 to 1.0 ppm in the finished product.

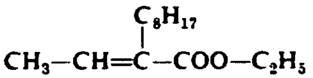
Prod.: from *n*-Oct-*1*-yne via its Sodio-derivative, with Ethyl chlorocarbonate to the Acetylenic ester.

G.R.A.S. F.E.M.A. No.2448.

4-17; 5-241; 103-295;

## 1318: ETHYL OCTYL CROTONATE

Ethyl-*alpha*-octyl-*alpha*-crotonate.
Ethyl-*2*-octyl-*2*-butenoate.



$CH_3{-}CH{=}C(C_8H_{17}){-}COO{-}C_2H_5$

$C_{14}H_{26}O_2 = 226.36$

Colorless or pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, oily and very tenacious odor, sweet in dilution, rather unpleasant when undiluted.

This ester, rarely offered under its proper chemical name, finds use in perfume compositions, not only in the herbaceous types, but also in heavy floral fragrances, where a warm-herbaceous undertone is desirable (Jasmin, Gardenia, Bouvardia, Tuberose, etc.).

Prod.: from Acetaldehyde by condensation with Decanal (Aldehyde C-10) followed by oxidation of the unsaturated C-12 aldehyde to the corresponding C-12 acid. The ethylester is subject material.

## 1319: ETHYL OCTYL KETONE

*3*-Undecanone.
Octyl ethyl ketone.

$CH_3{-}CH_2{-}CO{-}(CH_2)_7CH_3$

$C_{11}H_{22}O = 170.30$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Fruity, aldehydic-herbal odor, more fruity than Methyl nonyl ketone and less "Rue"-like.

Has been suggested for use in perfumery, but this ketone is not a common commercial item and does not offer any outstanding olfactory effects as compared to its homologues and isomers.

Prod.: by Grignard reaction on Ethyl Magnesium Chloride and Octyl chloride. Other methods are based upon Heptylmalonic ester reaction with Propionyl chloride.

31-81; 36-1143;

## 1320: ETHYL OCTYL-2-OXYACETATE

Ethyl octyl glycolate.

$C_8H_{17}—O—CH_2—COO—C_2H_5$

$C_{12}H_{24}O_3 = 216.32$

Colorless liquid. Slightly soluble in water, soluble in alcohol and oils.

More fruity and less floral, also less fatty than *n*-Octanol with respect to odor.

The taste is herbaceous-bitter in concentrations higher than 50 ppm. Rarely offered commercially, and probably of very limited interest. See notes under Methyl octyl-*2*-oxyacetate.

Prod.: from *n*-Octanol plus Ethyl diazoacetate.

31-158;

## 1321: ETHYL OENANTHATE

Not a well-defined, single chemical.
"Oenanthic ether".
"Cognac oil, artificial".

There are two types of "Oenanthic ether":

1) Mixed Ethyl-esters of the fatty acids isolated from Coconut oil by saponification.
2) A mixture of esters of Coconut fatty acids, prepared with alifatic alcohols from Methyl- to Octyl-.

Type 1) is the most common.

The esters include:

Ethyl heptoate
Ethyl octoate
Ethyl decylate
Ethyl dodecanoate
Ethyl tetradecanoate

and product 1) often contains traces of Amyl- and Heptyl alcohols.

It is a colorless oily liquid with a boiling range of about 170° to 290° C., mostly lower than 200° C.

This product is used occasionally in perfumery, e.g. in Citrus type fragrances and Citrus topnotes. It imparts a pleasant, natural, winey "mellow" note which blends excellently with the light Citrus notes.

Oenanthic ether is used extensively in flavor compositions, where it is sometimes preferred over Ethyl heptoate for its richer, rounder and more complex character.

It falls naturally into imitation Cognac, Brandy, Arak, Champagne, Wine, etc. as well as in many fruit flavors: Blackcurrant, Peach, Apple, Raspberry, Strawberry. It is an excellent modifier in flavors where Diacetyl and Acetylmethylcarbinol are present at high concentration, e.g. Butterscotch, etc.

G.R.A.S.

4-108; 77-187; 86-107; 95-182; 140-142;
see also: Ethyl heptoate.

## 1322: ETHYL OLEATE

Ethyl-*9*-octadecenoate.

$CH_3(CH_2)_7CH=CH(CH_2)_7—COO—C_2H_5$

$C_{20}H_{38}O_2 = 310.52$

Pale yellowish oily liquid, insoluble in water, miscible with alcohol and oils. Sp.Gr. 0.87. B.P. approx. 320° C (decomposition).

This ester may find a little use in perfumery as a solvent/modifier or a constituent of certain artificial flower absolutes, but its main use in that in flavor compositions.

When absolutely pure, it has very little odor, only a mild, sweet oily and warm – actually delicate fragrance. However, the ester decomposes slightly upon storage, causing harsh notes to appear and override the normal, delicate nuances.

The ester finds some use in Butter and fruit flavors, partly as a fixative, partly as an active flavor ingredient (mouthfeel, in Butter flavors), and it protects a flavor composition against the damaging treatment of oven-baking. The ester is therefore used in many flavor types for baked goods.

Concentration may vary from 0.1 up to 40 ppm in the finished product.

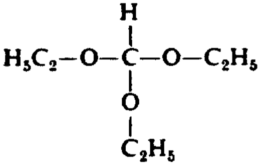
Prod.: by direct esterification of Ethanol with Oleic acid, using azeotropic conditions.

G.R.A.S. F.E.M.A. No.2450.

7-172; 26-548; 100-434; B-II-467;

## 1323: ETHYL ORTHOFORMATE

Aethon.
Triethoxymethane.



$$HC(OC_2H_5)_3$$

$C_7H_{16}O_3 = 148.21$

Colorless mobile liquid. Sp.Gr. 0.90.
B.P. 146° C.

Slightly soluble in water (under decomposition), soluble in alcohol and oils.

Sweet, somewhat camphoraceous-herbaceous odor with a Firneedle-like note.

Has been suggested for use in industrial fragrances for masking, etc. and may find some application in that field. It tends to lift the odor of the conventional components of a pine fragrance and increase the radiation, an effect often desirable for masking purposes.

Prod.: from Chloroform plus Ethanol plus Sodium ethoxide.

26-544; 66-554; 100-434; B-II-20;

## 1324: ETHYL OXYHYDRATE

Not a well-defined, single chemical.
"Rum ether".

A commercial name for a distilled product of mixed esters, alcohols, ketones and aldehydes.

The commercial product called "Rum ether" is available in many different types, some alcohol soluble, some oil-soluble and some are soluble in hydro-alcoholic mixtures.

Main components are:

| | |
|---|---|
| Water (not in oil-soluble types) | total minimum 99% |
| Ethyl alcohol | |
| Ethyl acetate | |
| Ethyl formate | |
| Acetone | |
| Acetaldehyde | |
| Methanol* | |
| Formaldehyde* | |

* total of these two chemicals must be less than 5%.

The entire product should distil below 100° C at atmospheric pressure, and leave no evaporation residue. There are, of course, commercial Rumethers of substantially different composition, some with significant amounts of higher boiling components.

Trace components include:
Furfural,
Diacetyl,
*iso*-Amyl alcohol and its esters (or "Fusel oil")
Decanoic acid and esters
Butyric acid and esters.

The conventional prescription for making "Ethyl oxy hydrate" may not produce these last mentioned materials. The product will contain a certain amount of water, which may be removed by redistillation (which unfortunately carries esters, etc. away in an azeotropic distillation) or by stirring with anhydrous Sodium sulfate. "Rum ether" of less than 10% water content is usually soluble in flavor oils and other oils.

"Rum ether" is used extensively in flavor compositions, not only in imitation Rum, but in a number of combination-flavors, such as Butterscotch, Vanilla, Cherry, Plum, Pineapple, Tutti-frutti, etc.

Concentrations may be about 60 to 400 ppm in icecream and candy, or up to 1600 ppm in alcoholic beverages.

G.R.A.S. F.E.M.A. No.2996.

See also: 4-17; 77-49; 77-50; 77-181; 104-565; 161-208; 140-134;

## 1325: ETHYL PALMITATE

Ethyl hexadecanoate.
Ethyl cetylate.

$CH_3(CH_2)_{14}COO—C_2H_5$

$C_{18}H_{36}O_2 = 284.49$

Colorless, needlelike crystals, melting at 25°C to a colorless, oily liquid, insoluble in water, soluble in alcohol, miscible with oils.
Sp.Gr. 0.86 (liquid). B.P. 303° C.

Very faint waxy odor, extremely mild, sweet.

Practically without taste, but produces a certain "creamy" mouthfeel.

Finds a little use in flavor compositions, mainly for imitation Butter and Rum. It also acts as a fixative for the very volatile components in these two types.

Concentration may be about 20 to 40 ppm in candy, sometimes higher in baked goods.

Prod.: directly from Ethanol and Palmitic acid by azeotropic type esterification.

G.R.A.S. F.E.M.A. No.2451.

26-548; 77-188; B-II-372; 66-587;

## 1326: ETHYL PENTADECANOATE

Ethyl pentadecylate.
Ethyl tetradecane-*1*-carboxylate.

$CH_3(CH_2)_{13}COO—C_2H_5$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Very faint, sweet odor, by some observers classified as "musky", others find the material virtually odorless.

It is quite possible that this material has very little odor when pure and isolated, but it is said to impart a sweetness and mellowness to fruit flavors, wine flavors, etc. which is normally obtained only by proper ageing.

The title ester has been identified in the volatile portion of wine.

The ester could find some use in flavor compositions, mainly in wine and fruit flavors, imitation Honey, etc.

Prod.: from (naturally occurring) Palmitic acid via Pentadecyl methylketone, by oxidation to Pentadecanoic acid, which is esterified to subject material.

158-186; B-II-370;

## 1327: ETHYL PENTIN CARBONATE

Ethyl-*n*-pent-*1*-yne carbonate.
Ethyl hexynoate.

$CH_3(CH_2)_2C\equiv C-COO-C_2H_5$

$C_8H_{12}O_2 = 140.18$

Colorless liquid. B.P. 188° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and penetrating, gassy-green, oily-vegetable odor of moderate to poor tenacity. In extreme dilution it displays quite pleasant and almost natural, sweet-green tonalities, and it could be classified as one of the more attractive Acetylenic esters. Several commercial products consist of mixtures of several esters, one of which is the title material.

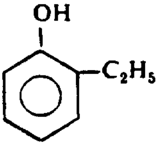
It has found some use in perfume compositions, not only as a Violet-leaf-green odor, but also as a trace component in fresh-green topnotes, where it blends excellently with Estragon and Basil. Its fate is, however, most conceivably the same as that of all the other Acetylenic esters: their days are numbered, and they can not stand up in competition with the modern and very natural Hexenyl and Nonenyl derivatives, etc.

Prod.: from Methyl-*n*-propyl ketone via *n*-Pent-*1*-yne to the acid and to the ester.

5-245;

## 1328: ortho-ETHYL PHENOL

*2*-Hydroxyethylbenzene.
*1*-Hydroxy-*2*-ethylbenzene.
Phlorol.
A minor component of rectified Birch tar oil (Creosote).



$C_8H_{10}O = 122.17$

Colorless liquid. Sp.Gr. 1.02. B.P. 207° C.

Slightly soluble in water, miscible with alcohol and oils.

Semi-sweet, tarry-medicinal odor, sweeter than that of phenol and more tar-like, smokey.

Warm and pungent taste, burning sensation unless highly diluted.

By those interested and experienced in the use of Birch tar products in perfumery, it is still considered most probable that the key fragrance notes of rectified Birch tar oil are to be found in the non-phenolic portion of the oil (the so-called non-saponifiable oil). The phenols in rectified Birch tar oil usually amount to 20 to 60% of the oil.

This statement was made as far back as in the early 1890's by the late perfumer and chemist J. Guerlain.

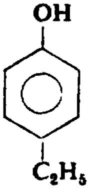
However, the subject phenol could find some use in the temporarily modern "leather"-like fragrance types for men, and in various bases requiring smokey or leather-like notes. The material carries with it the usual disadvantages of a phenol: tendency to discolor in daylight, and sensitivity to iron, alkali and air.

Prod.:
1) by isolation from Birch tar Creosote.
2) from *ortho*-Ethylbenzene sulfonic acid by alkali fusion.

26-548; 72-64; 100-808; 68-420; 104-99; B-VI-470;

## 1329: para-ETHYL PHENOL

4-Hydroxy ethylbenzene.
The *ortho*-isomer is also known (component of Birch tar Creosote).



$C_8H_{10}O = 122.17$

Needlelike crystals, colorless or white, turning yellowish-amber when exposed to daylight or iron. M.P. 48° C. B.P. 218° C.

Slightly soluble in water, soluble in alcohol, oils and aqueous alkali.

Powerful, woody-phenolic, medicinal, yet rather sweet odor. Sweeter than the Cresols, somewhat to the anisic type.

This phenol has been suggested for use in making artificial Castoreum and Mimosa bases. Castoreum has always been a comparatively inexpensive animal material, and is still available in reasonable quantity and quality, particularly as long as the beaver pelts are in demand as furs.

Mimosa, however, has its ups and downs, a winter freeze may kill many trees, a bush fire may wipe out other thousands of trees, and there are years of scarcity and very high prices, but the literature has little to say about the components of Mimosa. And the author is still waiting to see a really good artificial Mimosa base.

The Acetophenones and subject material certainly do not lend the delicate notes and softness which are among the typical features of Mimosa. Yet, the secret may be hidden in a few powerful trace ingredients, superbly fixed by Nature's own mild-smelling fixatives.

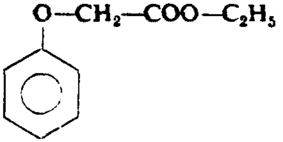
The author believes that subject material is only very rarely used in perfumery.

Prod.: from *para*-Ethylbenzolsulfonic acid by alkali fusion method.

7-106; 26-548; 90-381; B-VI-472; 72-64;

## 1330: ETHYL PHENOXY ACETATE

Phenoxyacetic acid, ethylester.



$C_{10}H_{12}O_3 = 180.21$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Sweet, somewhat honeylike, also floral odor of good tenacity. The honey-notes are less pronounced in this ester than in the conventional Ethyl phenylacetate, but the floral notes are more perceptible and tend to point in the Hyacinth direction.

Warm, sweet, honeylike taste.

This ester has been suggested for use in perfume compositions as a modifier for Ethyl phenylacetate, which is somewhat sharper and more pungent. The phenoxyacetate, however, has not found much interest for such purpose.

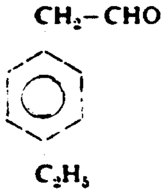
The ester is occasionally used in flavor compositions, mainly imitation Honey, where it can help tone down the rather pungent notes of the conventional Methyl- and Ethyl phenylacetates. Higher esters of Phenoxyacetic acid are also used in Honey – for perfumes and flavors, and some of them find their way into Styrax-bases.

Prod.: by direct esterification of Ethanol with Phenoxyacetic acid using azeotropic conditions. The acid can be obtained from Phenol plus Monochloroacetic acid in aqueous alkaline solution.

4-113;

## 1331: para-ETHYL PHENYLACETALDEHYDE

"Homo-syringa aldehyde" (sometimes called).



$C_{10}H_{12}O$ = 148.21

Colorless, slightly viscous liquid. Solidifies in the cold. Insoluble in water, soluble in alcohol and oils.

Somewhat gassy-earthy, but also floral odor, aldehydic-green, and, in suitable dilution, quite pleasant and sweet. Remotely reminiscent of the odor of crushed Lilac leaves.

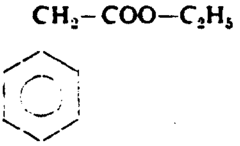
This aldehyde has been suggested for use in perfume compositions, mainly floral types, as part of a green complex or topnote complex. Its odor is softer, less pungent than that of the Methyl phenylacetaldehyde (Syringa aldehyde, so-called).

The author finds that this material is very rarely offered to the trade.

Prod.: (several methods): e.g. from *para*-Ethylbenzaldehyde plus Ethyl monochloroacetate to yield the glycidic ester. Saponification of the latter gives the aldehyde.

## 1332: ETHYL PHENYLACETATE

Ethyl-*alpha*-toluate.



$C_{10}H_{12}O_2$ = 164.21

Colorless liquid. Sp.Gr. 1.03. B.P. 229° C.

Insoluble in water, very poorly soluble in Propylene glycol, Glycerin, Mineral oil, soluble in alcohol, miscible with most perfume and flavor oils.

Powerful, sweet, Honey-like, slightly animal and quite persistant odor with a fruity undertone reminiscent of Apricot.

Sweet and fruity-honeylike taste at concentrations lower than 10 ppm.

Used in perfume compositions for its mildly animal notes, honey-character and power. In trace amounts, it may impart pleasant nuances in Muguet, Rose, Lily, Sweet Pea, Orange-blossom, Clover, Oriental bases and numerous types of "waxy" odor. In combination with lower alkyl cinnamates and in higher concentration, it creates the typical "low-cost Oriental" note.

In combination with lower alifatic Butyrates, certain Cresyl esters or ethers, it may sometimes create obnoxiously smelling bases after short time of ageing. It is a material of rather capricious character.

Very widely used in flavor compositions for imitation Honey, Apricot, Butter, Cherry, Peach, etc. and in tobacco flavorings.

Concentrations are usually low, about 2 to 10 ppm in the finished product, but may be as high as 25 ppm in syrups.

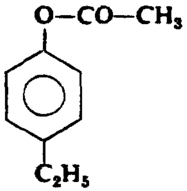
Prod.: from Benzyl cyanide and Ethyl alcohol with Sulfuric acid. The Benzyl cyanide may be produced directly from Benzyl chloride and Sodium Cyanide in a combination process.

G.R.A.S. F.E.M.A. No.2452.
FCC-1964-825.

4-17; 5-270; 26-548; 43-501; 44-245; 68-595; 77-194; 86-19; 95-185; 96-209; 100-434; 103-92; 106-152; B-IX-434; 140-151;

## 1333: para-ETHYL PHENYL ACETATE

Ethyl acetyl phenol.



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.

Harsh-anisic, rather powerful odor with sweet and somewhat floral character in higher dilution.

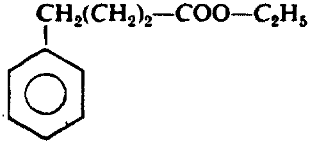
Has been suggested for use in perfume compositions, but this material does not have much to offer to the perfumer. The overall odor and performance is rather unattractive and pungent, and only mere traces can be useful in certain types of Cananga or Ylang-Ylang bases, etc.

Prod.: by Acetylation of *para*-Ethyl phenol with Acetic anhydride.

31-125;

## 1334: ETHYL PHENYL BUTYRATE

Ethyl-*4*-phenylbutyrate.
Ethyl-*gamma*-phenylbutyrate.



$C_{12}H_{16}O_2 = 192.26$

Colorless, slightly oily liquid. Insoluble in water, soluble in alcohol and oils.

Sweet, fruity, Plum-like odor of good tenacity.

Deep-sweet, fruit-jam-like taste, reminiscent of cooked Plums or Prunes.

This ester is probably used in flavors only. It imparts at very low concentration a certain amount of "natural" body and richness to many berry and other fruit flavors.

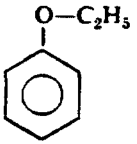
The concentration used in such flavors is equivalent to about 0.06 to 1 ppm in the finished products.

Prod.: by direct esterification of Ethanol with *gamma*-Phenylbutyric acid. The acid is obtained from Phenylbutyrolactone by reduction or from *gamma*-Bromopropylbenzene by Grignard reaction.

G.R.A.S. F.E.M.A. No.2453.

## 1335: ETHYL PHENYL ETHER

Phenylethyl ether.
Phenethole.
Ethoxybenzol.



$C_8H_{10}O = 122.17$

Colorless liquid. B.P. 172° C. Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils.

Pleasant, warm-aromatic, but somewhat pungent odor – more attractive in dilution.

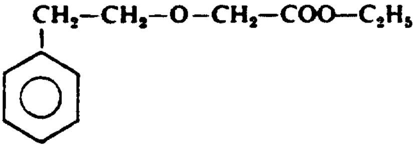
The lower homologue, Anisole, is used in industrial fragrances for masking, etc., and the title material has only a slightly better rating with the perfumers, apart from the fact that it is not nearly as common. Maybe the reason is, that the overall odor of Phenethole is rarely desired in any perfumery problem, and the notes extractable from this ether are not very unusual or interesting.

Prod.: from Phenol and Diethylsulfate in weak aqueous alkaline solution.

26-650; 68-426; B-VI-140;

## 1336: ETHYL PHENYLETHOXY ACETATE

Phenylethoxyacetic acid, Ethylester.



$C_{12}H_{16}O_3 = 208.24$

Colorless liquid. Very slightly soluble in water, soluble in alcohol and oils.

Rather harsh-rosy, semi-dry-odor of moderate to poor tenacity.

Oily-bitter, astringent taste and mouthfeel.

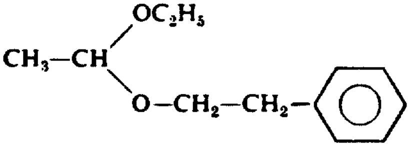
Although this material has been suggested for use in perfume compositions, the author feels that it has very little interest to the creative perfumer. The ester does not offer any unusual or very attractive notes, and a perfume laboratory does not really need it.

Prod.: by esterification of Ethanol with Phenylethoxyacetic acid.

31-158/159;

## 1337: ETHYL PHENYLETHYL ACETAL

Acetaldehyde-ethyl-phenylethyl acetal.
A mixed acetal.



$C_{12}H_{18}O_2 = 194.28$

Colorless liquid. B.P. 230° C.

Almost insoluble in water, soluble in alcohol, miscible with most perfume oils.

Leafy-green, delicately rosy and sweet odor of moderate tenacity.

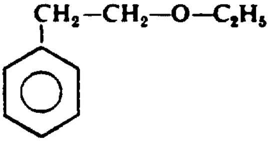
This Acetal is used in perfume compositions to introduce the green notes reminiscent of the calice, upper leaves and crushed flower stems of Rose and other flowers. It blends very well with the conventional Rose materials, and its earthy-floral-green character makes it particularly suitable for Hyacinth fragrances. It is much softer than the Phenylacetaldehyde and its relatives, and has a distinctly floral character. As an Acetal, it is more stable in soap and other mild-alkaline media, while it quickly deteriorates in acid liquid.

Prod.: from Acetaldehyde diethylacetal plus Phenylethyl alcohol (e.g. by short-time boiling).

5-321;

## 1338: ETHYL PHENYLETHYL ETHER

Phenylethyl ethyl ether.



$C_{10}H_{14}O = 150.22$

Colorless liquid. Practically insoluble in water, soluble in alcohol and perfume oils. Poorly soluble in Propylene glycol.

Very powerful, exotic-floral, pungent, sweet and warm odor of Hyacinth type with a Rose-like undertone. Rather poor tenacity.

This ether, which is the next higher homologue of an ether occurring in East Indian Pandanus oil (Kewda oil) has been developed in an attempt to find more lasting and softer smelling chemicals of that odor type.

It has found some use in heavy floral compositions, not only in the artificial Kewda oils – which are very popular in India – but also in Hyacinth, Narcissus, Wistaria, etc. or in fancy

Oriental bases. It needs very skilled fixation and it is often blended with other low-boiling, floral-woody odorants before being incorporated in the perfume or perfume base. Even modest amounts of Linalool seem to round off the roughness of this ether, and traces of Citral gives an often needed freshness. Styrax would be one of the preferred natural fixatives.

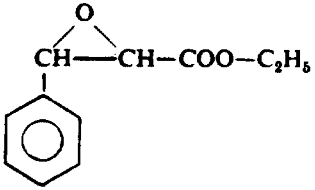
Prod.:

1) from Benzyl magnesium chloride plus Bromodiethyl ether.
2) from Phenylacetaldehyde diethylacetal by reduction in presence of a Nickel catalyst at 180° C.

See also: 104-504;
and: Ethyl-*ortho*-methoxybenzylether.
and: Methyl phenylethyl ether.

## 1339: ETHYL PHENYL GLYCIDATE

Ethyl-*3*-phenylglycidate.
E.P.G.
Ethyl-*alpha-beta*-epoxy-*beta*-phenylpropionate.



$C_{11}H_{12}O_3 = 192.22$

Colorless, slightly viscous liquid. Sp.Gr. 1.13.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Warm, caramellic-fruity odor, reminiscent of cooked Strawberries.

Sweet fruity-caramellic, "jam-like" taste, reminiscent of Strawberry and Plum preserves.

This ester finds a place in a number of perfume compositions, particularly those where a floral and fruity note is desirable, e.g. Jasmin and Gardenia, and also in many types of Lipstick perfume, where the conventional Ionone-type may need some modernization. It blends very well with the rose materials and with the Lactones, and it has a pleasant influence upon Benzylacetate and other sharp smelling materials.

It is used frequently in flavor compositions, not only in Strawberry, but quite widely in Berry imitation flavors, Tutti-frutti, Caramel, Treacle, Butterscotch, Maple-complexes, etc.

The concentration used is about 5 to 70 ppm in baked goods and other finished products, highest in gelatin desserts.

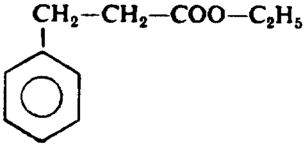
Prod.: from Benzaldehyde with Ethyl monochloroacetate, using Sodamide as condensing agent.

G.R.A.S. F.E.M.A. No.2454.
E.O.A. No.246.

68-926; 86-19; 106-153; 140-152;

## 1340: ETHYL-3-PHENYLPROPIONATE

Ethyl dihydrocinnamate.
Ethyl hydrocinnamate.



$C_{11}H_{14}O_2 = 178.23$

Colorless, somewhat oily liquid. Sp.Gr. 1.02. B.P. 240° C.

Almost insoluble in water, soluble in alcohol and oils, slightly soluble in Propylene glycol.

Sweet, very light, fruity-honeylike odor. Milder, more rosy-honeylike and more Hyacinth-like than the Methylester.

Sweet, fresh-fruity-floral taste with a honeylike note.

This ester finds use in many types of floral fragrance, e.g. Lilac, Rose, Appleblossom, Sweet Pea, etc. and in Oriental bases with Patchouli oil and Phenylacetates. Its fruity notes tend to appear Strawberry-like if the concentration is too high in a perfume base, but the ester can be advantageously utilized with the skilled combination of chemicals with a similar rate of evaporation.

In flavor compositions it can be used for various types of fruit and Honey complexes. It is also used in combination with Cinnamon and other spices for certain types of candy.

Due to the power of this material its concentration in the finished product is normally mere traces, e.g. 1 to 3 ppm.

Prod.:

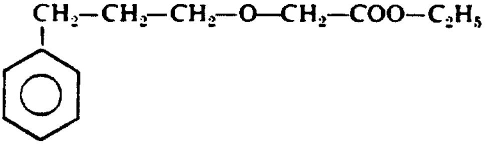
1) from Hydrocinnamic acid and Ethanol by normal esterification.
2) by hydrogenation of Ethyl cinnamate.

G.R.A.S. F.E.M.A. No.2455.

34-581; 4-16; 4-18; 86-18;

## 1341: ETHYL PHENYLPROPOXY ACETATE

Phenylpropoxyacetic acid, Ethylester.



$C_{13}H_{18}O_3$ = 222.29

Colorless oily liquid. B.P. 268° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-fruity and mildly balsamic odor with resemblance to Hydrocinnamic alcohol and Cinnamyl esters. Moderate tenacity.

With no really distinguished features or character, this material is not absolutely necessary for a perfumer to have in his daily or casual work. It would only have a place on the shelf if its price would be attractive enough to allow for its use at medium or high level of concentration, as a modifier in balsamic and fruity-sweet floral fragrance types, Oriental bases, etc.

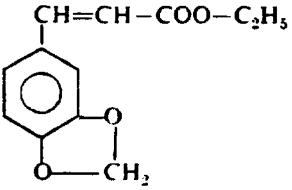
Prod.: from Phenylpropoxyacetic acid and Ethanol by esterification.

31-158,159;

## 1342: ETHYL PIPERONYL ACRYLATE

"Piperonylidene ethyl acetate".
"Ethyl piperonylidene acetate".

NOTE: The name "Ethyl piperonyl acetate" is sometimes applied to this material, probably because of confusion with the second synonym as listed above.



$C_{12}H_{12}O_4$ = 220.23

Colorless or white crystals. M.P. 68° C.

Almost insoluble in water, soluble in alcohol and oils.

Very faint, sweet-herbaceous odor of good tenacity. The material tends to produce "cinnamic" notes upon standing or due to poor storage conditions.

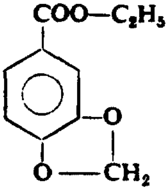
Although repeatedly mentioned in perfume literature, the subject ester does not seem to have created any interest among perfumers. Its effect is too weak, its overall odor value insignificant.

Prod.: from Heliotropine and Malonic ester, using Piperidine catalyst to yield Piperonyl acrylic acid, which is esterified to subject material.

47-45;

## 1343: ETHYL PIPERONYLATE

Ethyl-*3,4*-methylene dioxybenzoate.
"Tagetol".



$C_{10}H_{10}O_4 = 194.19$

Colorless, slightly viscous liquid. Sp.Gr. 1.24.

Practically insoluble in water, soluble in alcohol and oils.

Powdery-herbaceous and slightly fruity odor of good tenacity. The trade name "Tagetol" for this ester is, in the author's opinion, rather pretentious because the unprepared observer of the material will undoubtedly expect more "natural" Tagetes odor out of it – if he is at all familiar with Tagetes-oil or absolute. There is no "Apple-like" odor, and no intense greenness, but there is a deep herbaceous and very lasting, semi-dry, powdery note which could be classified as part of the Tagetes picture.

The ester has found a little use in perfume compositions, mainly for fantasy notes, new variations of "powdery" notes, etc., and in certain types of "tabac" fragrances, With proper support of Clary sage and Linalyl- og certain "Carbinyl"-esters it can supply a Tea-like effect of some interest.

Prod.: by oxidation of Heliotropine with Potassium permanganate to produce the acid, from which the ester is made by conventional methods.

The acid is also obtained directly from Safrole.

4-18; 4-131; 28-609; 86-20;
See also: Ethyl piperonyl acrylate, Methyl piperonylate.

## 1344: ETHYL PROPIONATE

Ethyl propanoate.
Propionic ether.

$C_2H_5—COO—C_2H_5$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. B.P. 99° C.
Sp.Gr. 0.89.

2% soluble in water, miscible with alcohol, perfume and flavor oils. Vapors form explosive mixtures with air – flammable material.

Very volatile, ethereal, fruity-rum-like odor.

Sweet, fruity-ethereal, rum-like taste. The flavor effect in aqueous media is weak. The fruity taste is reminiscent of Apple and Banana.

The ester is occasionally used in perfumery to introduce an "aged" topnote in the alcoholic perfume solutions, particularly for Citrus-colognes, etc.

Widely used in flavor compositions for imitation Rum, Arak, Apple, Banana, Pear, Pineapple, Plum, Butter, Butterscotch, Tutti-frutti (or juicy-fruit) and numerous other types.

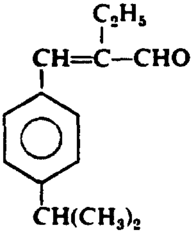
The concentration is usually very high, since the ester is a weak flavor material, about 10 to 100 ppm in candy or baked goods, and up to 1100 ppm in chewing gum.

Prod.:
1) by direct esterification of Ethanol with Propionic acid under azeotropic conditions.
2) from Ethanol and Propionic anhydride.
3) from Ethanol vapors and Propionic acid vapors at 230° C over a catalyst.

G.R.A.S. F.E.M.A. No.2456.

4-18; 5-230; 43-501; 43-620; 44-806; 77-184; 86-20; 100-435; 103-90; 160-1188; B-II-240; 140-137;

## 1345: alpha-ETHYL-para-iso-PROPYL CINNAMIC ALDEHYDE



$C_{14}H_{18}O = 202.30$

Pale yellowish or almost colorless oil.
B.P. 267° C. Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Warm, sweet, winey-Rum-like odor of good tenacity.

Has been suggested for use in perfume compositions, mainly as a variant and modifier for the green-floral and herbaceous aldehydes of related structure, some of which are commonly used perfume chemicals.

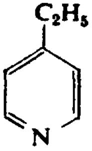
However, this aldehyde has not achieved much popularity among perfumers and it is most conceivable that it will remain a more or less "forgotten" material.

Prod.: by condensation of *n*-Butyric aldehyde and Cumin aldehyde.

93-151;

## 1346: 4-ETHYL PYRIDINE

4-Homopicoline.
*gamma*-Homopicoline.



$C_7H_9N = 107.16$

Colorless or pale straw-colored or pale amber-colored oily liquid. B.P. 165° C.

Very slightly soluble in water, soluble in alcohol and oils.

Very powerful, sweet-green, in the pure state nauseating, in dilution slightly minty odor with sweet-herbaceous, mildly tarry-pungent undertones. There is a certain similarity to the odor of mushrooms and dry-rotted wood. In suitable dilution actually a pleasant odor.

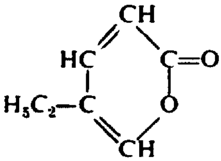
This alkyl-substituted Pyridine could find use in perfume compositions since it gives very interesting effects with Vetiver, Oakmoss, Hydroquinone dimethylether, Amylsalicylate, Coumarin, Lavender, etc., and in minute traces in certain florals, e.g. Hyacinth and Tuberose. Also for "bouquetting" purposes in floral fragrances describing flowers from the floor of the woods, Muguet, Violet, etc. where the sweet-earthy, fungal notes can be applied artistically with pleasant effect.

Prod.: (several methods) e.g. by Wolff-Kishner reduction of 4-Acetylpyridine.

69-524;
Sample: Reilly Tar & Chemical Corp., Indianapolis, U.S.A.

## 1347: 5-ETHYL-alpha-PYRONE

Ethyl coumalin.
5-Ethyl-2-pyrone.



$C_7H_8O_2 = 124.14$

Colorless oily liquid. Slightly soluble in water, soluble in alcohol and oils.

Sweet haylike, breadlike odor.

Somewhat burning, warm-bread-like taste, pleasant in extreme dilution. The author believes that this material is used in certain perfume specialties. This comparatively rare chemical has been suggested for use in flavor compositions, e.g. to participate in the reconstitution of the flavor in bread and fried potatoes and certain other processed foods.

The subject chemical is commercially available from suppliers other than the manufacturers of perfume and flavor chemicals.

Prod.: from Malic acid via Coumalic acid.

69-819;

## 1348: ETHYL PYRUVATE

Ethyl acetyl formate.
Ethyl ketopropionate.
Ethyl-*2*-oxopropanoate.
Ethyl pyro-racemate.

$CH_3—CO—COO—C_2H_5$

$C_5H_8O_3 = 116.12$

Colorless liquid. Sp.Gr. 1.06. B.P. 155° C.

Slightly soluble in water, miscible with alcohol and oils.

Sweet floral-fruity, warm odor of poor tenacity.

Sweet, warm and slightly spicy-caramellic taste with a trace of a fruity note.

This ester has found some use in perfumery where powerful sweet, fruity-floral topnotes are desirable, e.g. in Cassie bases. It needs considerable fixation, but it blends well with the Anisyl esters or Anisates for the above purposes.

It is used in flavor compositions for imitation Caramel, Maple, Brandy, Arak, Rum, Butterscotch, Treacle, Chocolate, and in spice blends and fruit complexes.

Concentration is normally about 20 to 150 ppm in the finished product.

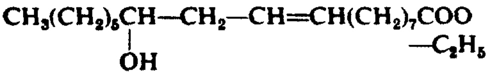
Prod.: by direct esterification of Ethanol with Pyruvic acid using azeotropic conditions.

G.R.A.S. F.E.M.A. No.2457.

5-240; 7-173; 160-1206; 26-550; B-III-616; 86-20; 66-862; 140-149;

## 1349: ETHYL RICINOLEATE

Ethyl-*12*-hydroxy-*9*-octadecenoate.
Ethyl oxyoleate.



$CH_3(CH_2)_5\underset{\substack{|\\ OH}}{CH}—CH_2—CH{=}CH(CH_2)_7COO—C_2H_5$

$C_{20}H_{38}O_3 = 326.52$

Pale yellowish viscous oil. Sp.Gr. 0.91. B.P. 363° C.

Insoluble in water, soluble in alcohol and oils.

Very faint "oily" odor when pure. Less sweet, more harsh-smelling if poorly stored or oxidized.

Occasionally used in perfume compositions, mainly as a component of artificial flower absolutes, etc. or in various places to introduce a natural oily note of lasting effect.

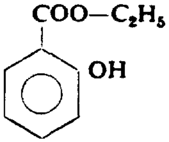
The ester is also used in flavor compositions for a similar purpose.

Prod.: by direct esterification of Ethanol with Ricinoleic acid.

4-18; 86-20;

## 1350: ETHYL SALICYLATE

Ethyl-*ortho*-hydroxybenzoate.
*2*-Hydroxy ethylbenzoate.
"Sal ethyl".
"Salicylic ether".



$C_9H_{10}O_3 = 166.18$

Colorless oily liquid, solidifying in the cold, melting at about 1° C. Sp.Gr. 1.13.
B.P. 234° C.

Slightly soluble in water, soluble in alcohol miscible with oils.

Heavy, sweet, floral-fruity odor, milder than Methyl salicylate, more Cassie-like, more intensely sweet-floral undertones.

Used in perfume compositions for Cassie-bases, Ylang-Ylang, Lily and many other sweet florals. Also in traces as a sweetener in Fougères, etc.

Sweet and heavy-fruity taste, not burning at same concentration as Methylsalicylate.

The ester is used in flavor imitations of Blackberry, Blackcurrant, Gooseberry, Raspberry, Strawberry, etc. and in fruit complexes, in so-called "root beer" or "Sassafras" types and as a modifier for Methyl salicylate in dentifrice flavors and Wintergreen flavors in general.

Concentration is normally limited to mere traces, except in certain types of dentifrice and chewing gum, where it may be as high as 1000 ppm.

Prod.: by direct esterification of Ethanol with Salicylic acid- preferably under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2458.

4-18; 26-550; 43-501; 44-788; 61-74; 77-193; 86-20; 95-188; 96-207; 100-435; 103-92; 106-154; 160-1220; B-X-73; 140-150;

## 1351: ETHYL SORBATE

Ethyl-2,4-hexadienoate.
Ethyl-2-propenyl acrylate.

$CH_3—CH=CH—CH=CH—COO—C_2H_5$

$C_8H_{12}O_2 = 140.18$

Colorless liquid. B.P. 185° C.

Slightly soluble in water, soluble in alcohol, miscible in oils.

Warm-fruity and somewhat ethereal odor.

Fruity-caramellic, slightly winey taste.

This ester is used in flavor compositions, mainly imitation fruit flavors, and particularly for baked goods where its flavor type and relative stability are advantageous.

The concentration used is about 5 to 20 ppm in baked goods.

Prod.: by direct esterification of Ethanol with Sorbic acid, e.g. under azeotropic conditions.

The acid is obtained from Crotonaldehyde plus Malonic acid.

G.R.A.S. F.E.M.A. No.2459.

66-645;

## 1352: ETHYL STEARATE

Ethyl octadecanoate.

$CH_3(CH_2)_{16}COO—C_2H_5$

$C_{20}H_{40}O_2 = 312.54$

Solid crystalline mass, melting at 34° C.
B.P. 318° C. Sp.Gr. 0.85 (liquid).

Insoluble in water, soluble in alcohol, miscible with most oils.

Virtually odorless when pure.

Very faint waxy taste (or rather mouthfeel).

This ester is occasionally used in flavor compositions where a waxy taste (or mouthfeel) is desirable, e.g. in imitation Honey or in certain types of chocolate flavor.

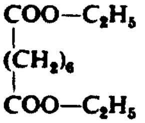
The concentration used varies considerably with the purpose and the end-use of this ester.

Prod.: by esterification of Ethanol with Stearic acid. The acid is obtained from Oleic acid by hydrogenation, a method which yields comparatively pure Stearic acid, free from Palmitic acid.

26-550; 77-188; 100-436; 160-1226;
B-II-379;

## 1353: ETHYL SUBERATE

Ethyl octane dioate.
Diethyl suberate.



$$\begin{array}{l} COO-C_2H_5 \\ | \\ (CH_2)_6 \\ | \\ COO-C_2H_5 \end{array}$$

$C_{12}H_{22}O_4 = 230.31$

Colorless liquid, insoluble in water, soluble in alcohol and oils. Sp.Gr. 0.98. B.P. 285° C.

Sweet, deep, fruity odor of berry-like character.

Somewhat tart, astringent, but pleasant-fruity, berry-and-jam-like taste. Some observers find it similar to that of Mulberry.

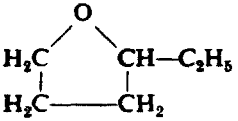
The ester is NOT listed in the American Federal Register as G.R.A.S. but the author believes that Ethyl suberate is used by the flavor industry in a number of countries.

Prod.: by esterification of Ethanol with Suberic acid. The acid is obtained in the process known as "cracking" of Castor oil.

31-126; 160-1230;

## 1354: 2-ETHYL TETRAHYDROFURAN

*2*-Ethyl tetramethylene oxide.



$C_6H_{12}O = 100.16$

Colorless mobile liquid.

Slightly soluble in water, soluble in alcohol and oils.

Powerful and diffusive, sweet-herbaceous odor with a woody undertone.

Relatively poor tenacity.

Bitter taste in concentrations as low as 20 ppm.

This material has been made commercially available most likely for the purpose of offering a more complete range of trace ingredients in (artificial) essential oils. Several alkyl-substituted Tetrahydrofurans have been identified in Nature, and many are available to the perfumer or flavorist.

It may find use in artificial Mint oils, but its use should not be confined to such limited areas, since it gives interesting effects with Lavender, Pine Needle, etc. in low-cost household product fragrances, etc.

Prod.: by chlorination of Tetrahydrofuran (an industrially available chemical) followed by Grignard reaction with Ethyl magnesium bromide.

It can also be prepared from Furfural.

See also: 69-163;
See: Heptyl tetrahydro furan.
*2,4*-Diethyl tetrahydrofuran.
Hexyl acetyl tetrahydrofuran.

## 1355: ETHYL THIOGLYCOLATE

Ethyl mercaptoacetate.

$HS-CH_2-COO-C_2H_5$

$C_4H_8O_2S = 120.17$

Colorless oily liquid. Sp.Gr. 1.11.
B.P. 158° C.

Almost insoluble in water, soluble in alcohol and oils.

The odor of this ester has been described as "onion-like", but the author believes, based upon personal studies, that a good commercial grade of this ester has little or no such odor. The odor may be slightly herbaceous, green-fruity, and not exceptionally pleasant.

Apart from being a possible ingredient in cosmetic preparations, this ester is probably not being used in perfume or flavor formulations.

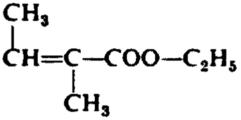
The obnoxious odor of "sulfide" may occur during oxidation to which all the thiol-substituted acids are very sensitive. The oxidation produces the corresponding Disulfides. This odor may enter during the preparation of the acid which in turn carries the sulfide odor to all its esters.

The use of high-grade Thioglycollic acid is, therefore, of imperative importance in solving the odor problem connected with all Thioglycollates.

34-1245; 66-807;

## 1356: ETHYL TIGLATE

Ethyl-*trans-2*-methyl-*2*-butenoate.
Ethyl-*trans-2*-methylcrotonate.
Ethyl-*trans-2,3*-dimethylacrylate.



$\overset{CH_3}{\overset{|}{C}}H=\underset{\underset{CH_3}{|}}{C}-COO-C_2H_5$

$C_7H_{12}O_2 = 128.17$

Colorless liquid. B.P. 156° C. Sp.Gr. 0.93.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-ethereal, fruity odor of deep, slightly caramellic note.

Caramellic-fruity, "jam-like" taste.

Finds some use in perfumery in the creation of unusual topnotes, particularly for the non-floral fragrance types. The higher esters of Tiglic acid are often preferred for their better lasting qualities. The ester is also used in the reproduction of certain essential oils.

Ethyl tiglate is used in flavor compositions for imitation Raspberry, Strawberry, Pineapple, Rum, Butterscotch, etc.

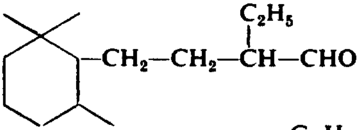
The concentration used is normally about 5 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2460.

Prod.: by direct esterification of Ethanol with Tiglic acid.

4-18; 66-636;

## 1357: alpha-ETHYL-2,2-6-TRIMETHYLCYCLOHEXANE BUTYRIC ALDEHYDE



$C_{15}H_{28}O = 224.39$

Pale straw-colored or almost colorless, slightly viscous liquid. Insoluble in water, soluble in alcohol and oils, very poorly soluble in Propylene glycol.

Sweet, somewhat woody, but overall floral-ambre-like odor with a peculiar "fishy" undertone, resembling that of Allyl Ionone.

This aldehyde has been suggested for use in perfume compositions several decades ago, and it was developed in an attempt to find new and interesting Ionone derivatives.

The material is not commercially available under its proper chemical name, but several European manufacturers have marketed specialties under trade names, and based these partly or entirely upon the title chemical.

Its tenacity and relative stability makes it a potential soap perfume chemical, but its market price is still too high for such purpose on a larger scale.

Prod.: from Tetrahydro methylionone by condensation (Darzen's type reaction) with Ethyl monochloroacetate, followed by saponification of the glycidic ester.

See also: 31-53;

# 1358: ETHYL UNDECIN CARBONATE

Ethyl undecyne carbonate.
Ethyl dodecynoate.

$CH_3(CH_2)_8C{\equiv}C—COO—C_2H_5$

$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. B.P. 273° C.

Insoluble in water and Propylene glycol, soluble in alcohol and oils.

Fatty, sweet-earthy, green and Reseda-like odor, weaker or milder than Ethyl decincarbonate, and not as closely resembling Reseda. Good tenacity.

The title acetylenic ester has little, if any interest to the perfumer at all. Its lack of power is disappointing, particularly in consideration of its cost. It is included in this work mainly for the sake of completing the monographs on the acetylenic esters, many of which are now obsolete or about to become so.

Prod.: from Methyl nonyl ketone via *n*-Undec-*1*-yne to the acid, from which the Ethylester is prepared.

3-16; 4-18;

# 1359: ETHYL UNDECYLATE

Ethyl hendecanoate.
Ethyl undecanoate.

$CH_3(CH_2)_9—COO—C_2H_5$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid. B.P. 255° C.
Sp.Gr. 0.87.

Insoluble in water, soluble in alcohol, oils and Propylene glycol.

Winey-fatty-fruity and somewhat nut-like odor.

Sweet-oily, slightly fruity taste.

This ester – often confused with Ethyl undecylenate – see next monograph – is probably not very common in perfumes or flavors. The author believes, that the name Ethyl undecylate often refers to Ethyl undecylenate, which is much more common and less expensive.

However, the subject ester could be used in perfumes for its pleasant Cognac-type note, as a part of a topnote complex, in Citrus Colognes, Chypres and modern fruity-aldehydic complexes.

Its winey Cognac-like flavor could be utilized in imitation Cognac flavors and various fruit flavors.

Prod.: by direct esterification of Ethanol with Undecylic (Undecanoic) acid, using azeotropic conditions.

7-173; 26-550; 35-854; 103-91; B-II-358;
See also: Ethyl undecylenate (next).

# 1360: ETHYL UNDECYLENATE

Ethyl-*10*-undecenoate.
Ethyl-*10*-hendecenoate.

$H_2C{=}CH(CH_2)_8COO—C_2H_5$

$C_{13}H_{24}O_2 = 212.34$

Colorless oily liquid. B.P. 264° C.
Sp.Gr. 0.88.

Insoluble in water, soluble in alcohol and oils. Somewhat soluble in Propylene glycol.

Pleasant fruity-winey odor, more winey than Undecylic ester, and less floral (see previous monograph).

Oily-winey, slightly fruity taste.

This ester is used in perfume compositions as part of the floral complex in Cassie, Jasmin, Rose, Violet, Ylang-Ylang, Tuberose and in Oriental fragrance types, etc. It has a softening effect upon the conventional (and often sharp or harsh) topnote materials, and it blends well with the finer grades of Citrus oils, particularly Bergamot and Bitter Orange.

It is also used in flavor compositions, e.g. for imitation Cognac, Brandy, Rum, Coconut, Quince and in Fruit and Nut complexes.

It is a comparatively powerful flavor chemical, and the concentration in finished products may be as low as 1 to 10 ppm. Together with higher alifatic esters of Undecenoic acid it forms part of the more powerful oil-soluble types of Rum ether, so-called.

Prod.: by direct esterification of Ethanol with Undecenoic acid under azeotropic conditions.

The acid is obtained in the pyrolysis of Castor oil.

G.R.A.S. F.E.M.A. No.2461.

4-18; 35-851; 86-20; 77-188; 66-638; 140-145;

## 1361: ETHYL VALERATE

Ethyl pentanoate.
Ethyl-*n*-valerianate.
NOTE: The commercial product is most often the Ethyl-*iso*-valerate (see next monograph).

$CH_3(CH_2)_3—COO—C_2H_5$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. B.P. 145° C.
Sp.Gr. 0.87.

0.25% soluble in water, soluble in alcohol and Propylene glycol, miscible with perfume and flavor oils.

Powerful and diffusive, ethereal-fruity, Apple-like odor with a remote resemblance to Pineapple. Esters with traces of free acids will show this very perceptibly in the odor, not so conspicuously in the flavor (in aqueous media).

Sweet and somewhat pungent-fruity, Apple-like, almost "gassy"-ethereal taste. In extreme dilution, the taste is merely sweet fruity.

Very rarely used in perfume compositions. The ester is very susceptible to hydrolysis and – as above mentioned – its odor very sensitive to traces of free acid.

Widely used in flavor compositions, mainly for Apple imitations, but also for Apricot, Peach and in Butter and Nut complexes. Its power is utilized in the "Tutti-frutti" type of flavor for chewing gum, and it is occasionally used in tobacco flavoring.

Concentrations vary from 5 to 15 ppm in the finished product, and up to 250 ppm in chewing gum.

Prod.: by direct esterification of Ethanol with *n*-Valeric acid preferably under azeotropic conditions. It is important that the ester is absolutely dry (free from water).

NOTE: With a flash point of about 27° C the ester presents a certain fire hazard and its vapors may form explosive mixtures with air at high room temperature.

G.R.A.S. F.E.M.A. No.2462.

31-124; 43-501; 43-933; 90-199; 100-437; 160-1274; B-II-312; 140-141;
See also: B-II-301;
– and the following monograph: Ethyl-*iso*-valerate.

## 1362: ETHYL-iso-VALERATE

Ethyl-*beta*-methylbutyrate.
Ethyl-*iso*-pentanoate.
Ethyl-*iso*-valerianate.
"Ethyl valerate" (commercial *iso*-valerate is often called so).

$(CH_3)_2CH—CH_2—COO—C_2H_5$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. B.P. 135° C.
Sp.Gr. 0.87.

0.3% soluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Powerful, diffusive and penetrating-ethereal, vinous-fruity odor. In extreme dilution sweet, Apple-like fruity.

Sweet-fruity, Apple-like taste in proper dilution. The presence of traces of free acid is detrimental to the odor of this ester, but it is of minor importance to the flavor in aqueous media, since this flavor chemical is normally used in conjunction with acid.

Very rarely, if ever, used in perfume compositions.

Widely used in flavor compositions for Fruit complexes, tobacco flavorings, imitation Apple, Pineapple, Cheese, Rum and in various Nut complexes, particularly Walnut and Black Walnut.

Concentration in candy may vary from 5 to 30 ppm, while in chewing gum it may be as high as 450 ppm.

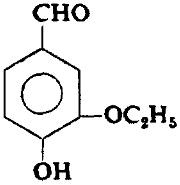
Prod.: by direct esterification of Ethanol with *iso*-Valeric acid under azeotropic conditions. It is important for the stability of the ester that it is absolutely dry.

G.R.A.S. F.E.M.A. No.2463.

4-18; 26-550; 43-932; 77-186; 86-20; 90-200; 100-432; 103-91; 160-1068; B-II-312;

## 1363: ETHYL VANILLIN

Protocatechualdehyde-*3*-ethylether.
(The commercial name "Ethylvanillin" is misleading).
*3*-Ethoxy-*4*-hydroxybenzaldehyde.
*3*-Ethoxy protocatechualdehyde.
NOTE: See monograph: ETHYL VANILLIN, following *iso*-Ethyl vanillin after this monograph.
An enormous number of trade names include: Ethovan – Ethyvan – Ethylprotal – Vanillodor – Bourbonal – Rhodiarome – Vanillal – Vanillose – Vanillum – Vanirone – Vanisol – Novovanillin – Quatrovanil – Protethyl – Supervanil – Vanillarom – Vanillodin – Vanillidine (a mixture) – etc. etc.



$C_9H_{10}O_3 = 166.18$

White or creamy-white crystal needles, flakes or crystalline powder. M.P. 78° C.

Slightly soluble in water (about 1%), soluble in alcohol, diluted alsohol, Propylene glycol, diluted Propylene glycol, and in most perfume and flavor oils.

Intensely sweet odor, warm, slightly floral and with some resemblance to Vanilla in its creamy sweetness. The tenacity is outstanding, and the odor power only demonstrated in dilutions of this chemical.

Intensely sweet, warm, creamy-Vanilla-like taste. The flavor power is often given at 4 times that of Vanillin, but most flavorists agree that it is actually about 2 to 2½ times stronger than Vanillin, and with a different odor-and-flavor type.

This aldehyde is widely used in perfumery as a sweetener and fixative, not only in very sweet type floral fragrances and the conventional fruity lipstick-type fragrances, but in general as part of the fixative element in perfume compositions where a creamy sweetness is desirable, particularly in combination with florals such as Ylang-Ylang, or with all members of the Eugenol family in Carnations, etc.

Ethyl vanillin is often used to substitute a larger amount of Vanillin in a fragrance when a discoloration problem arises, due to the active hydroxyl- or aldehyde-groups of the Vanillin/Ethylvanillin molecules. The discoloration hazard can be reduced and the sweetness maintained although there will be a loss in physical fixation effect.

This aldehyde is used very extensively in flavor compositions, mainly in imitation Vanilla, also in Chocolate, "Cream-Soda", Butterscotch, and in almost any type of fruit flavor, Caramel, Nut, etc. as well as Rum, Butter, etc. as a sweetener, fixative and "amplifier" to the flavor composition. It performs very well with Acetylmethyl carbinol and Diacetyl for the latter purpose.

For Vanilla imitation flavor it is mostly used in combination with Vanillin and/or other derivatives of Protocatechu aldehyde since Ethyl vanillin alone does not properly express the natural Vanilla note.

Concentrations amount to 20 to 200 ppm under normal circumstances in various types of consumer products, except in Chocolate toppings where it may run as high as 4000 ppm.

As an example, the concentration in "Imitation Vanilla Extract" may be about 28,000 ppm – but this product is not consumed as such.

G.R.A.S. F.E.M.A. No.2464.

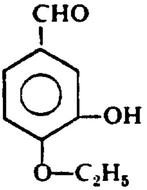
Prod.:

1) by Ethylation of Protocatechualdehyde. This method yields also *iso*-Ethylvanillin, see next monograph.
2) from Catechol monoethylether by treatment with Chloroform and Sodium hydroxide.
3) a process similar to the making of Vanillin from Guaiacol uses *ortho*-Ethoxyphenol to be condensed with Chloral. The condensation product is oxidized with Potassium hydroxide in Methanol and subsequently acidified to liberate the Ethylvanillin. The product is usually purified by distillation under vacuum with heated condensers (about 80° C).

4-18; 4-122; 5-133; 26-550; 29-423; 68-747; 77-206; 85-31; 86-20; 95-146; 100-437; 103-170; 106-155; B-VIII-256; 140-164;

## **1364:** iso-**ETHYL VANILLIN**

*3*-Hydroxy-*4*-ethoxy benzaldehyde.
Protocatechualdehyde-*para*-monoethyl ether.
"*iso*-Bourbonal".



$C_9H_{10}O_3$ = 166.18

White crystals, melting at 126° C.

Slightly soluble in water, soluble in alcohol, Propylene glycol and most perfume and flavor oils.

Sweet, somewhat floral odor, remotely reminiscent of Vanilla, but much weaker than Ethyl vanillin (see previous monograph), and also weaker than Vanillin.

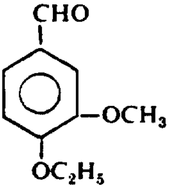
This aldehyde was developed in line with many other derivatives of Protocatechu aldehyde in search of better and more true-to-Nature Vanilla chemicals. Its lack of power and the fact that it is not prepared from such low cost starting materials as is Vanillin, contribute to the failure of its success as an Aroma chemical.

Prod.: e.g. by mono-ethylation of Protocatechualdehyde. This process yields a certain amount of Ethyl vanillin, too.

68-747; 140-279;

## **1365: ETHYL VANILLIN** (chem. name)

NOTE: This monograph describes the chemical the correct name of which is: Ethyl vanillin.
*3*-Methoxy-*4*-ethoxybenzaldehyde.
Protocatechu aldehyde methyl ethyl ether.
"Homo veratraldehyde" (sometimes called).



$C_{10}H_{12}O_3$ = 180.21

White or colorless prismatic crystals or crystalline powder. M.P. 65° C.

Sweet, somewhat floral odor, remotely reminiscent of Vanilla, more so than commercial "Ethyl vanillin", but not with the same strength.

Sweet Vanilla-like taste of approximately two times the power effect of Vanillin.

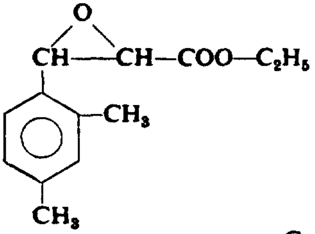
Has been suggested for use in flavor composition as a modifier for Vanillin and Ethyl vanillin (commercial). In spite of its more natural Vanilla-like flavor, it has a disadvantage of higher manufacturing cost, since it is most conveniently made from Vanillin.

Prod.: by Ethylation of Vanillin with Diethyl sulfate in aqueous alkaline solution.

61-62; 68-747; 72-149;

## 1366: ETHYL XYLYL GLYCIDATE

The commercial product consists of a mixture of isomers, mainly *meta-*:
Ethyl-*alpha-beta*-epoxy-*beta*-(*2,4*-dimethylphenyl)-propionate.



$C_{13}H_{16}O_3 = 220.27$

Colorless or pale straw-colored, oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-fruity and slightly floral odor, the fruity notes being more Cherry-and-Plum like, while the floral undertone is Jasmin-like.

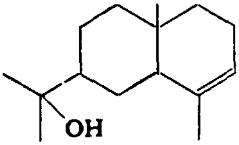
This peculiar odor has tempted some perfumers to use the material experimentally in Jasmin and other fruity-floral compositions. Its tenacity is good, but its lack of character puts a rather low limit to the level of use of the material.

The ester is rarely offered under its proper chemical name.

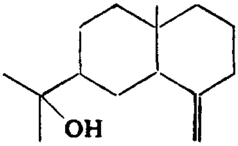
Prod.: from *2,4*-Dimethyl benzaldehyde plus Ethyl chloroacetate plus Sodamide or Sodium ethylate as condensing agent.

## 1367: EUDESMOL

"Selinenol".
Commercial product is a mixture of *alpha-* and *beta*-forms:



*alpha*-Eudesmol
M.P. 82° C.



*beta*-Eudesmol
M.P. 76° C.

$C_{15}H_{26}O = 222.37$

White or pale yellowish crystalline mass (crude commercial material) or white crystals.

Insoluble in water, soluble in alcohol, miscible with most oils.

This alcohol has found some use as a fixative for woody, floral and spicy fragrance types.

Its very delicate, sweet-woody and warm notes tend to be floral in combination with more volatile components. In that respect it resembles Farnesol, but it does not have the beauty of that alcohol. Eudesmol is very tenacious and blends well with almost any type of conventional perfume material.

Prod.: by isolation from Araucaria oil, or by isolation from the "tail" fractions of various Eucalyptus oils.

17-47; 88-268; 104-71;
see also Eudesmyl acetate.

## 1368: EUDESMYL ACETATE

$C_{15}H_{25}—OOC—CH_3$

$C_{17}H_{28}O_2 = 264.41$

(Structure: see Eudesmol).

Pale yellowish, viscous liquid. B.P. 264° C.
Sp.Gr. 0.99.

Sweet, fruity, slightly floral odor, reminiscent of Pear or Bergamot. The tenacity is exceptionally good.

This ester is used in perfume compositions where a Linalylacetate-type odor of greater tenacity is desired. In fact, the ester was used during and after World War II as a substitute/modifier for Linalyl acetate. At that time the ester was available at an advantageous price, well below that of Linalyl acetate.

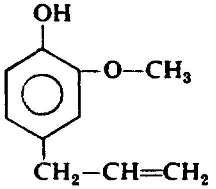
Today, the cost of Linalyl acetate (synthetic) is so low, that not even the Australian Eudesmyl acetate can compete with it. Only the superior tenacity and therefore better fixation obtained with the subject material can keep it on the market. A steady production of various Eucalyptus oils is almost necessary to entertain a production of Eudemol and its esters.

Prod.: by acetylation of Eudesmol (see previous monograph).

88-273; 104-72;

## 1369: EUGENOL

*2*-Methoxy-*4*-allyl phenol.
*4*-Allylguaiacol.
*4*-Allyl-*2*-methoxyphenol.
*4*-Hydroxy-*3*-methoxy-*1*-allylbenzene.
*4*-Allylcatechol-*2*-methylether.
Carygenol.
Eugenic acid.
Phyllol (trade name, confusing).



$C_{10}H_{12}O_2 = 164.21$

Colorless or very pale straw-colored oily liquid.

Very slightly soluble in water, miscible with alcohol and oils, soluble in Propylene glycol and in dilute aqueous alkali. Viscosity and color increase with age and exposure to air and daylight. B.P. 253° C. Sp.Gr. 1.07.

Powerful, warm-spicy, rather dry and almost sharp odor, drier and harder than that of Clove bud oil, less peppery-woody than that of Clove leaf oil.

Warm-spicy taste, somewhat burning unless highly diluted. The taste is usually followed by a warm mouthfeel, then a burning sensation, delay and sequence depending upon the acidity or alkalinity of the saliva. Pungency depends upon the concentration of Eugenol.

Extensively used in perfume compositions, conventionally in Carnation, for which purpose the author would recommend *iso*-Eugenol in spite of the almost unanimous use of Eugenol in published formulations. For incense, Oriental fragrances, Rose bases, certain types of Fougère, "Blue-Grass" type fragrances, etc. and in all variations of modern Spice types, Eugenol is commonly used in large amounts.

For flavors, this phenol is used not only in spice complexes, but also as a modifier in Mint flavors, Nut flavors, various fruit complexes, and rare flavors such as date, etc.

Eugenol is in no way a substitute for Clove bud oil in flavors, but it may add to the strength and give a clove-like note to combination-spice flavors.

Concentrations in finished consumer products range from 10 to 100 ppm in candies and baked goods, up to 200 ppm in meat products and up to 500 ppm in chewing gum. It may reach the same level in toothpaste, but is normally lower than 300 ppm in oral products.

G.R.A.S. F.E.M.A. No.2467.

Prod.: by isolation from Clove leaf oil, or Clove stem oil, or Cinnamon leaf oil, occasionally from Bay leaf oil or from Clove bud oil.

With a Clove leaf oil price of U.S. $ 2.20 to 3.30 per kilo (1967-1968) there is no interest in promoting synthetic methods of making Eugenol. This phenol remains one of the most important perfume and flavor chemicals exclusively made from natural sources by simple isolation (alkali wash). Clove leaf oil has been extremely stable in price until late 1967 when it increased significantly over a period of 1968. Even the subsequently higher prices for all Eugenol products have not encouraged the research on an economical method of making Eugenol from a "non-natural" source.

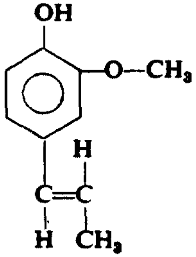
Synthesis: One method uses Guaiacol as a starting material. Although Guaiacol is present in wood tar, it is most conveniently prepared from Catechol (Pyrocatechol) by Monomethylation. Catechol is obtained from Phenol which is a coal tar derivative. When Guaiacol is reacted with Allyl chloride the Guaiacol allylether can be rearranged to Eugenol.

The production of Eugenol from Coniferyl alcohol – widely distributed in the plant Kingdom – is of no immediate importance.

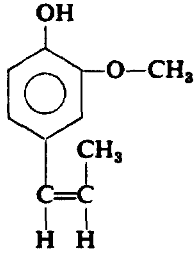
4-49; 5-275; 34-1115; 44-806; 68-973; 77-198; 86-51; 85-61; 90-430; 100-439; 106-156; 156-160; B-VI-961; 140-170;

## 1370: iso-EUGENOL

*2*-Methoxy-*4*-propenyl phenol.
*4*-Propenylguaiacol.
*iso*-Carygenol.
Propenyl-*ortho*-cresol methylether.
The commercial product is a mixture of *cis*- and *trans*-isomers:



*trans-iso*-Eugenol.
M.P. 33° C. B.P. 266° C.
Normally 82 to 88% of commercial *iso*-Eugenol.



*cis-iso*-Eugenol.
Liquid. B.P. 262° C.
Normally 12 to 18% of commercial *iso*-Eugenol.

$C_{10}H_{12}O_2 = 164.21$

The description below refers to commercial *iso*-Eugenol:

Sp.Gr. 1.09 solidifies in the cold, melts at approximately 13° C.

Pale yellowish or almost colorless, slightly viscous liquid, practically insoluble in water, soluble in alcohol, oils and Propylene glycol, soluble with turbidity in mineral oil, insoluble in Glycerin.

Mild and sweet, deep-floral ,very tenacious odor with great warmth and resemblance to Carnation, Sweet Williams or Wallflower. Poorer grades often show variable degree of dry-woody Eugenol-spiciness.

Warm, sweet, slightly burning taste with a floral note and spiciness varying with the quality of the material.

Extensively used in perfume compositions, mainly as a base for Carnation, but also in general as a sweet floralizing agent of excellent tenacity. It has the same sensitivity to alkali as Eugenol has, and it has a somewhat greater tendency to polymerize. Polymerization is accompanied by loss of odor and increase in viscosity and color. The subject material is therefore not recommended for soap perfumes. It can be used in modest amounts and in other than white soaps.

*iso*-Eugenol is a classical ingredient in "l'Origan" type fragrances and it may give the highly desirable warm background and powdery note in a Lilac base. It finds its way into numerous perfume bases and finished fragrances, artificial essential oils (Ylang-Ylang, Nutmeg, etc.) and enjoys a position – although not unique – that there are no substitutes for *iso*-Eugenol in perfumes.

It is used sparingly in many types of flavor, e.g. imitation Raspberry, Peach, Nutmeg (Mace), Cinnamon, Apricot, as well as in fruit complexes, Nut, Mint, Spice bases and in Clove flavors.

Concentration is normally only a few ppm in the finished product, except in chewing gum where it may reach 1000 ppm.

G.R.A.S. F.E.M.A. No.2468.
FCC-1964-845.

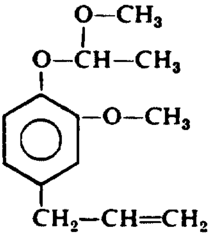
Prod.: from Eugenol by isomerization with alkali under heat. Potassium hydroxide is usually applied. The quality of *iso*-Eugenol varies considerably from one supplier to another, but the commercial products all have in common that the *trans*-isomer is the chief component. Perfumers do not quite agree which isomer is the most desirable one, and until a clear agreement is achieved, there is little chance that the method of production will be changed in such a way that one isomer can be favored.

4-71; 5-276; 34-1116; 68-975; 77-198; 86-74; 90-442; 106-206; 26-552; 156-160; B-VI-955; 140-171;

## 1371: EUGENOL METHYL ACETAL

Acetaldehyde eugenyl methyl acetal.
A mixed acetal of Eugenol and Methanol upon Acetaldehyde.

**Note**: It has been claimed that commercial products under this name are compositions and do not represent a single chemical. The description below refers to the chemical Eugenol methyl acetal.



$C_{13}H_{18}O_3 = 222.29$

Pale straw-colored liquid. Almost insoluble in water, soluble in alcohol and oils.

Dry spicy-green odor, more reminiscent of Bayleaf than of Clove.

Has been suggested for use in perfume compositions as a modifier for Eugenol and its conventional derivatives. It has also been claimed than subject chemical is stable and non-discoloring in mildly alkaline media (e.g. soap). However, it is commonly agreed that Eugenol owes its power and distinct spiciness to the presence of a free Hydroxyl-group. As soon as it is occupied (Methoxy- or Acetyl- or Sodium- etc.) the typical spice odor diminishes or disappears.

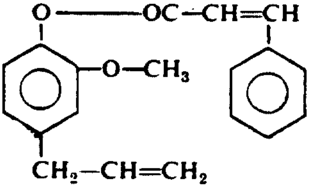
Subject acetal, like many other acetals, owes its spiciness to the presence of small amounts of free Eugenol, while the acetal itself probably lends the greenness and peculiar dry notes.

Very rarely offered commercially.

Prod.: from Acetaldehyde dimethylacetal and Eugenol.

## 1372: EUGENYL CINNAMATE

Eugenol cinnamate.
Cinnamoyl eugenol.



$C_{19}H_{18}O_3 = 294.35$

Needle-like crystals, white or colorless.
M.P. 91° C. Sp.Gr. 1.01 (liquid). B.P. 292° C.

Insoluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and in most perfume oils.

Virtually odorless and tasteless when pure. However, most commercial lots show a faint balsamic-spicy odor. The effect is more perceptible when this material is brought into use in combination with more volatile materials.

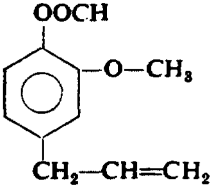
Its low volatility makes it suitable as a physical fixative, but this material produces some amount of odor in compositions. It may increase the richness of Oriental, Spice or Carnation type fragrances without changing the overall odor picture. It also serves as a fixative in Cinnamon compositions where the most active ingredients are rather volatile, and in various types of Clove compositions.

Prod.: from Cinnamoyl chloride and Eugenol sodium.

34-1116; 86-31; 100-440;

## 1373: EUGENYL FORMATE

Eugenol formiate.
*4*-Allyl-*2*-methoxyphenyl formate.



$C_{11}H_{12}O_3 = 192.22$

Colorless or very pale yellowish oily liquid. Sp.Gr. 1.12. B.P. 270° C.

Almost insoluble in water, soluble in alcohol and oils, somewhat soluble in Propylene glycol.

Warm-woody, somewhat dry odor with a remote resemblance to Orris and a fresh-spicy, slightly green undertone.

The taste is warm, somewhat dry, woody and remotely spicy.

This comparatively rare chemical is occasionally used in perfume formulations when variations in the conventional spice theme are desirable. It blends well with the woody notes, but not so attractively with the floral types.

Eugenyl formate finds a little use in flavor compositions as part of various types of spice blends. The concentrations used is normally limited to mere traces.

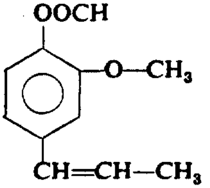
Prod.: by formylation of Eugenol.

G.R.A.S. F.E.M.A. No.2473.

34-1115; 103-86;

## 1374: iso-EUGENYL FORMATE

*2*-Methoxy-*4*-propenyl phenyl formate.
*4*-Propenyl-*2*-methoxyphenylformate.



$C_{11}H_{12}O_3 = 192.22$

Colorless or pale straw-colored slightly viscous liquid. Sp.Gr. 1.12. B.P. 282° C.

Almost insoluble in water, soluble in alcohol and oils. Slightly soluble in Propylene glycol.

Fresh-green, sweet-woody, almost Orris-like odor with an unquestionable Clove-like undertone.

It should be kept in mind that Formates of Phenols of this type rarely come on the market in high chemical purity. An odor description is therefore very subjective and dependent upon the origin of the sample of subject material.

This chemical finds a little – but probably very little – use in perfume compositions, often in combination with the Ionones e.g. in l'Origan-type fragrances, etc.

G.R.A.S. F.E.M.A. No.2474.

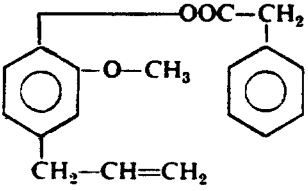
Prod.: by formylation of *iso*-Eugenol.

34-1116; 103-175;

## 1375: EUGENYL PHENYLACETATE

Eugenol phenylacetate.

(Often confused with *iso*-Eugenol phenylacetate which is the more common of the two).



$C_{18}H_{18}O_3 = 282.34$

Pale straw-colored, viscous liquid. B.P. 320° C. Sp.Gr. 1.15.

Insoluble in water, soluble in alcohol and oils.

Mild, but warm and sweet, slightly spicy odor of excellent tenacity. There are honey-like tonalities in most of the commercial products, but there are also products in which that note is absent or hardly perceptible. Trace surplus of Phenylacetic acid is not uncommon in very highboiling esters of that acid.

This material is occasionally used in perfume compositions as a modifier in Carnation bases, where a particularly delicate and discrete Spice-note is desirable, and *iso*-Eugenol does not cover the full olfactory picture. However, the *iso*-Eugenyl ester is generally preferred over this material.

It finds some use in Lilac bases where it may introduce the warm and rich undertones, often difficult to obtain.

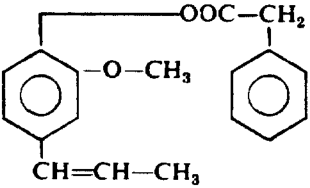
Prod.: from Phenylacetyl chloride and Sodium eugenol.

4-50; 34-247; 86-51;

## 1376: iso-EUGENYL PHENYLACETATE

*4*-Propenylguaiacyl phenylacetate.

*2*-Methoxy-*4*-propenylphenyl phenylacetate.



$C_{18}H_{18}O_3 = 282.34$

Pale yellowish, viscous liquid. Sp.Gr. 1.15.

Insoluble in water, soluble in alcohol and oils.

Intensely sweet, Vanilla-Clove-like odor, overall warm and mild, but extremely tenacious and with Honey-tobacco-like undertones.

Sweet-spicy, somewhat Vanilla-like, slightly fruity taste in proper dilution (less than 5 ppm).

This material has found some use in perfume compositions as a Carnation modifier and fixative, as well as in Honey and "Tabac" type bases, in certain types of Lilac and other delicate florals. Its very low volatility makes it suitable as a physical fixative, and its delicate odor (when reasonably pure) makes it applicable at comparatively high concentration (4-6-8 %) in the proper bases.

It is used in trace amounts in various Spice blends and imitation fruit and Honey flavors, particularly those intended for baked goods.

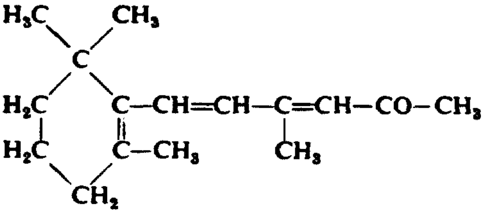
G.R.A.S. F.E.M.A. No.2477.

Prod.: from Phenylacetyl chloride plus *iso*-Eugenolsodium.

34-248; 34-1116;

## 1377: beta-EUIONONE

*2*-Methyl-*4*-(*1*,*1*,*3*-trimethyl-*2'*-cyclohexen-*2'*-yl)-butadiene methylketone.
*4*-Methyl-*6*-(*1*,*1*,*3*-trimethyl-*2'*-cyclohexen-*2'*-yl)-*3*,*5*-hexadien-*2*-one.



$C_{16}H_{24}O = 232.37$

Almost colorless or pale straw-colored oily liquid.

Semi-sweet, woody and slightly fruity, warm odor of good tenacity and some resemblance to *beta*-Ionone, but more sweet, less woody than that material.

This ketone has been suggested for use in perfume compositions as being superior to *beta*-Ionone with respect to overall odor performance and versatility in use.

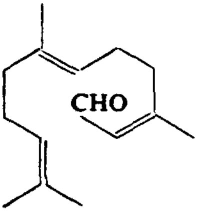
However, the manufacture of this material is somewhat more costly than that of the Ionones, at least as long as no one can set up a truly large scale production of this chemical. There is also some doubt that it can replace, let alone outperform, any of the common Ionones as far as odor quality is concerned.

Prod.: from Citral and *iso*-Propylidene acetone by condensation followed by cyclization.

31-95; 86-51; 86-78;
See also: Ianthone.

## 1378: FARNESAL

*2,6,10*-Trimethyl-*2,6,10*-dodecatrien-*12*-al. The commercial product is normally a mixture of several stereo-isomers.



$C_{15}H_{24}O = 220.36$

Colorless or very pale straw-colored liquid.
B.P. 268° C. (variable for the isomers).
Sp.Gr. 0.91.

Insoluble in water, soluble in alcohol, oils and Propylene glycol.

Very mild, sweet-oily, slightly woody, tenacious odor.

The aldehyde itself has very little to offer to the creative perfumer, but it opens the door for the perfume chemist to make Tetrahydro farnesal or Nor-hexahydrofarnesal, two very interesting floral perfume materials.

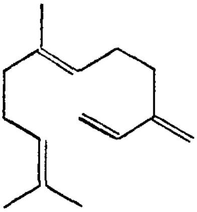
Farnesal is produced from

1) Cabreuva oil, from which Nerolidol is isolated by distillation. Oxidation with $CrO_3$ yields Farnesal.
2) from synthetic Nerolidol (Roche process).

2-1006; 4-50; 67-663; 86-51; 88-237; 89-121;

## 1379: FARNESENE

*2,6,10*-Trimethyl-*2,6,9,11*-dodecatetraene.



$C_{15}H_{24} = 204.36$

Colorless mobile liquid.

Insoluble in water, poorly soluble in alcohol, soluble in most perfume oils.

Very mild, sweet and warm, rather nondescript odor of good tenacity.

Apart from some possible use in the reconstruction of certain essential oils, there is, to the author's knowledge, very little, if any, use for this Sesquiterpene in perfumery as such.

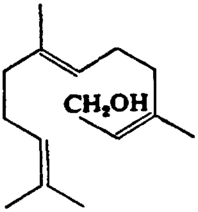
Prod.:

1) by dehydration of Farnesol by heat with a dehydrating agent.
2) from Nerolidol by heat with Acetic anhydride.

87-228; 100-443;

## 1380: FARNESOL

*2,6,10*-Trimethyl-*2,6,10*-dodecatrien-*12*-ol.



$C_{15}H_{26}O = 222.37$

Colorless oily liquid. B.P. 263° C.
Sp.Gr. 0.89.

Insoluble in water, soluble in alcohol, perfume and flavor oils and in Propylene glycol.

Very mild and delicate, sweet-oily odor, slowly developing a floral fresh-green note, reminiscent of certain notes from Muguet. The tenacity is outstanding, but the material as such tends to develop a different odor if it is exposed to air for longer time (blotter test).

This sesquiterpene alcohol has long been known and admired by perfumers who often wished they could have the material available at a reasonable cost. It was not intil late in 1967 that one manufacturer made the chemical available at a cost where it could truly be said that it is now everybody's perfume material, no longer reserved for the most costly fragrances.

Farnesol forms an excellent background note and blender in the delicate floral such as Muguet, Lilac, etc. or in the balsamic types, Oriental fragrances, Chypres etc. It combines the softest woody notes of Orris with the sweet and balsamic floral notes of Muguet, Rose, Magnolia, Acacia, etc. It blends excellently with YlangYlang, Cassie, Rose, Violet, Neroli, Cyclamen, etc. and it is an almost necessary ingredient in the so-called "Linden-blossom" type fragrance.

Its flavor is hardly enjoyed unless the material is incorporated in a flavor formulation. It will lend richness and stability and soft background to many fruit types, such as Apricot, Banana, Berry, Cherry, Citrus, Gooseberry, Melon, Peach, Raspberry, Strawberry, etc.

The concentration used may be as low as 0.1 ppm in the finished product, but in certain types of product it may reach 2 ppm or even more.

G.R.A.S. F.E.M.A. No.2478.

Prod.: (synthetic): from Acetylene via Methylbutynol – Methylheptenone – Dehydrolinalool – Linalool – Geranyl acetone – Dehydronerolidol – Nerolidol – Farnesol.
or from natural Nerolidol from Cabreuva oil: by treatment with Acetic anhydride to Farnesyl acetate. Saponification yields Farnesol.

4-50; 31-20; 31-30; 67-662; 77-173; 86-52; 88-233; 100-443; 106-159; 140-127;

## 1381: FARNESYL ACETATE

Structure formula see Farnesol (previous monograph).

$C_{15}H_{25}—OOC—CH_3$

$C_{17}H_{28}O_2 = 264.41$

Colorless oily liquid. B.P. 268° C.

Insoluble in water, soluble in alcohol, oils and Propylene glycol.

Very faint odor, somewhat green-floral, remotely rosy.

This ester has found a little use in perfume compositions for the fixative portion of Rose bases, etc.

It also finds some use in flavor compositions for imitation Apple, Gooseberry, etc. and in various herbal flavors.

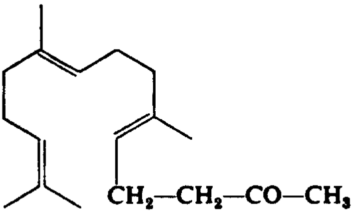
The flavor of Farnesyl acetate is hardly perceptible until the ester is incorporated in a flavor composition. Its effect is mainly that of "rounding-off" and producing a mellowing background, but it does have a faint, fruity-green taste in proper dilution.

Prod.: by Acetylation of Farnesol, or rather by treatment of Nerolidol with Acetic anhydride.

4-51; 77-173; 77-183; 86-52;

## 1382: FARNESYL ACETONE

*6,10,14*-Trimethyl-*5,9,13*-pentadecatrien-*2*-one.



$C_{18}H_{30}O = 262.44$

Colorless or pale straw-colored oily liquid. Sp.Gr. 0.98. B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Intensely sweet, floral and creamy-winey odor of excellent tenacity.

This ketone has been suggested for use in perfume compositions, but its use has so far been limited by the comparatively high price of the material.

It could find use as a fixative in floral compositions, Oriental bases, etc. It blends particularly well with Ylang Ylang and related odors, it lends good fixation to Jasmin and Tuberose, and gives delicate undertones in a Magnolia.

Prod.:

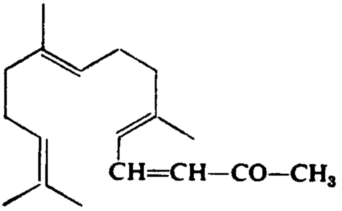
1) from Farnesol via Farnesyl chloride – Ethyl farnesyl acetoacetate – by hydrolysis and decarboxylization to the title material.
2) from Nerolidol plus Ethyl acetoacetate with Sodium Ethylate catalyst.

It has also been prepared by regulated hydrogenation of Farnesylidene acetone.

86-52;

## 1383: FARNESYLIDENE ACETONE

*6,10,14*-Trimethyl-*3,5,9,13*-pentadecatetraen-*2*-one.



$C_{18}H_{28}O = 260.42$

Colorless or pale straw-colored oily liquid. Sp.Gr. 0.90. B.P. over 300° C.

Almost insoluble in water, soluble in alcohol and oils. The material tends to deteriorate upon standing, become darker of color, more viscous, less sweet-floral of odor.

Ethereal-floral, rich and sweet odor of considerable tenacity. The odor suffers considerably when the material is exposed to air, daylight or heat.

This material has been suggested for use in perfume compositions as a novel part of floral complexes, even part of floral-green topnote complexes. However, the variations in odor observed in materials of different origin and age, and the obvious instability of the ketone has greatly discouraged perfumers from using or even trying the material in new creations. It is no longer regularly available.

See also: Farnesyl acetone.

Prod.: by heating of Farnesol with Acetone and Aluminum *iso*-propylate in Benzene under Nitrogen blanket.

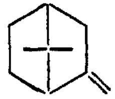
86-52; 88-238; 89-124;

## 1384: FENCHENE

At least seven isomers and stereo-isomers are known.

*l-alpha*-Fenchene is probably the best known.

*alpha*-Fenchene:



$C_{10}H_{16} = 136.24$

*alpha*-Fenchene: B.P. 155° C. Sp.Gr. 0.87.
*beta*-Fenchene: B.P. 152° C. Sp.Gr. 0.86.

Colorless mobile liquid. Insoluble in water, soluble in alcohol and perfume oils.

Fresh, Camphor-like odor of poor tenacity. Somewhat sweeter than Camphor, also slightly cooler.

If this Monoterpene could become available at a low cost, it might find its way into a number of masking odors for industrial perfumery purposes, and in a number of new artificial essential oils.

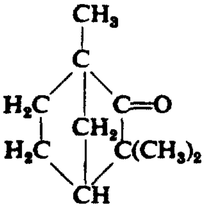
Prod.:

1) by dehydration of Fenchyl alcohol. The resulting "mixed Fenchenes" may be the commercial product.
2) by dehydration of *alpha*-Fenchyl alcohol. This yields *alpha*-Fenchene.
3) The terpene can also be obtained by isolation from various essential oils.

4-51; 67-622; 67-627; 87-199;

## 1385: FENCHONE

*laevo*-Fenchone. (*dextro-* is known but less common as a fragrance material).
*1,3,3*-Trimethyl-*2*-norbornanone.
*1,3,3*-Trimethyl bicyclo-*1,2,2*-heptanone-*2*.



$C_{10}H_{16}O = 152.24$

Colorless mobile liquid. Solidifies in the cold, melts at 6° C. B.P. 193° C. Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils.

Warm-camphoraceous, powerful and diffusive, basically sweet odor.

Warm, somewhat burning and bitter taste with a medicinal note.

This ketone finds some use as a masking odor in industrial fragrances. It is also used in the reconstruction of Fennel oil and a few other essential oils.

In spite of its rather unpleasant taste, it is used in various Berry complex flavors, in Spice complexes and in certain types of Liqueur flavoring.

The concentration used is about 0.1 to 5 ppm in the finished product.

Prod.:

1) by isolation from Cedarleaf oil ("Thuja" oil).
2) by various synthetic methods.

G.R.A.S. F.E.M.A. No.2479.

4-51; 67-619; 89-330;

## 1386: FENCHYL ACETATE

*1,3,3*-Trimethyl-*2*-norbornanyl acetate.
Structure formula – see: Fenchyl alcohol.

$C_{10}H_{17}—OOC—CH_3$

$C_{12}H_{20}O_2 = 196.29$

Colorless mobile liquid. Sp.Gr. 0.98.
B.P. 220° C.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Mild, rather sweet Fir Needle oil type odor, somewhat milder than Bornyl acetate, and not quite as characteristic, conifer-like.

This ester has been marketed with the intention of making it a modifier for Bornyl acetate (or rather *iso*-Bornyl acetate), but it does not have the power of the above conventional esters, and it has never been priced as low as *iso*-Bornyl acetate.

The ester still finds some use in fragrances for household products, etc.

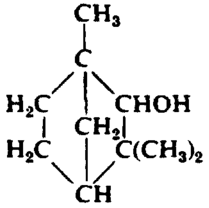
Prod.: by Acetylation of Fenchyl alcohol.

4-51; 36-481;

## 1387: FENCHYL ALCOHOL

*1,3,3*-Trimethyl-*2*-norbornanol.
*1,3,3*-Trimethyl bicyclo-*1,2,2*-heptanol-*2*.
*2*-Fenchanol.
Fenchol.

NOTE: The odor description below refers to commercial grade *alpha*-Fenchyl alcohol.



$C_{10}H_{18}O = 154.25$

Solid crystalline mass, colorless, translucent, occasionally pale straw-colored.
M.P. (*dextro*-Fenchol): 48° C.,
*laevo*-Fenchol: 49° C.

The racemic *alpha*-Fenchol has a somewhat lower melting point, and the *beta*-Fenchols are all liquid at room temperature.

Fenchol made by reduction of Fenchone from Cedarleaf oil is usually a mixture of several isomers, including the crystalline *alpha*-isomers. The *beta*-isomer forms a crystalline Hydrate which may be solid at room temperature.

Almost insoluble in water, soluble in alcohol, miscible with oils. Powerful and diffusive, Camphor-like, but sweeter and more Citrus-like almost Lime-like odor with more or less of an earthy-dry character, according to the composition and isomer-ratio.

The taste is somewhat bitter-Lime-like, camphoraceous and slightly woody-musty.

This interesting alcohol (or mixed alcohols) finds use in perfume compositions ranging from woody or herbaceous to Citrus-Lime and even certain floral types. It produces power and "lift" to floral fragrances, and solid background to Lime and other Citrus bases, having the advantage over the Terpenes in being very stable in soap.

Fenchyl alcohol is also used in flavor compositions such as Strawberry and other berries, Lime and Spice, etc.

The concentration is normally low, e. g. 0.2 up to 5 ppm in the finished product.

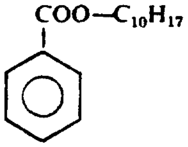
Prod.: by reduction of Fenchone, which may be derived from Cedarleaf oil or from other natural sources, or prepared synthetically from Pine terpenes. One French manufacturer uses Hydration of Turpentine under acid conditions to produce the alcohol.

G.R.A.S. F.E.M.A. No.2480.

4-51; 67-619; 88-192;

## 1388: FENCHYL BENZOATE

Structure formula: see Fenchyl alcohol.



$C_{17}H_{22}O_2 = 258.36$

Colorless viscous oil. Sp.Gr. 1.05.

Insoluble in water, soluble in alcohol, miscible with most oils.

This rare ester finds a little use in perfumery as a fixative in Pine and woody fragrance types, in certain Fougère types and low-cost Oriental fragrances.

It is generally considered true, that the ester is virtually odorless when absolutely pure, but the rare commercial lots are probably far from pure. They carry significant amounts of by-products from the peculiar and complex reaction by which the ester normally is prepared.

Prod.: directly from Pinene with Benzoic acid under certain catalytic conditions and at elevated temperature (150° C.).

86-52; 88-198;

## 1389: FENCHYL-n-BUTYRATE

Structure formula – see Fenchyl alcohol.

$CH_3—(CH_2)_2—COO—C_{10}H_{17}$

$C_{14}H_{24}O_2 = 224.35$

Colorless liquid. Sp.Gr. 0.96.

Mild and sweet-herbaceous odor with some resemblance to overripe fruit. Also reminiscent of fresh Valerian root (free from the obnoxious odor of acid from aged roots).

Sweet and herbaceous, somewhat spicy taste.

This ester, only rarely offered, has been suggested for use in perfume compositions as a modifier in sophisticated Pine fragrances, Cypress odors, etc. for room sprays etc.

However, it does not keep very well, since the acid notes seem to appear in all but the very fresh batches of this chemical, and accordingly, the ester has not become popular at all.

Prod.: from Pinene by hydration including the use of *n*-Butyric acid.

4-51;

## 1390: FENCHYL-iso-BUTYRATE

Structure formula – see Fenchyl alcohol.

$(CH_3)_2CH—COO—C_{10}H_{17}$

$C_{14}H_{24}O_2 = 224.35$

Colorless liquid. Sp.Gr. 0.95.

Fresh-herbaceous, slightly Conifer-like odor of moderate tenacity. It bears some resemblance to the odor of fresh Valerian root – but less so than the *n*-butyrate.

Slightly fruity, sweet-herbaceous taste with a root-like undertone.

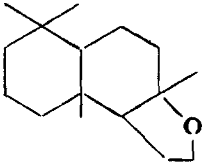
Although this ester keeps better than the *n*-butyrate, it has never become a common or popular material and is rarely offered commercially. It could probably find some use in household fragrances, etc.

Prod.: by hydration of Pinene including *iso*-Butyric acid in the acid treatment.

4-51;

## 1391: FIXATEUR 404

A trade name for:
*3a*-Methyl-dodecahydro-*6,6,9a*-trimethyl-naphtho-*(2,1-b)*furan.
or: Dodecahydro-*3a,6,6,9a*-tetramethyl-*(2,1-b)*-furan.



$C_{16}H_{28}O = 236.40$

Very viscous, colorless liquid.

Insoluble in water, soluble in alcohol, miscible with most perfume oils. Poorly soluble in Propylene glycol.

For several decades, this was the only true-to-Nature Ambergris chemical available to the creative perfumer. Several specialties were prepared with this chemical as the carrying or strongly supporting note, and although its identity has been revealed a few years ago, it still maintains a leading position among the comparatively few, truly powerful and natural Ambergris chemicals.

Its odor is not very impressive at first – or when undiluted. But when properly diluted, preferably incorporated and well mellowed in a composition, it shows its exceptionally powerful, yet delicately dry, woody-Ambergris-like, extremely tenacious odor.

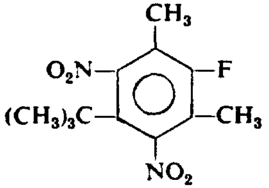
Its use in perfumery is not confined to that of being a part of an Ambergris base. It is an outstanding fixative for many types of fragrance, for all the Ionones and many Oriental bases, for the modern fruity-aldehydic fragrances, where Galbanum plays an important role in the dry topnote theme and prolonged green middle note, etc. Its normal dosage in a perfume composition may be about 0.1 to 0.2%, but great variations can be found; effects are perceptible at much lower concentrations, and interesting effects can be obtained at much higher concentration. Its delicate and discrete note makes it applicable even in floral fragrance, where normally dry smelling chemicals would cause problems. Often appearing at the very beginning, along with the topnote of the perfume, it remains pleasantly perceptible until the very end of the terminal notes.

Prod.: (several methods): e. g. from Manool or Sclareol, two isolates from natural oils. It has also been produced from isolated components of natural Ambergris. Such method naturally leads to unreasonably expensive end products. The current price of Fixateur 404 is approximately half of the market price for average grade Ambergris.

88-366; 156-367; (see also Firmenich publications and data, technical booklet).
See also: Ethyl dodecahydro trimethyl naphthofuran.

## 1392: 2-FLUORO-4,6-DINITRO-1,3-DIMETHYL-5-tertiary-BUTYLBENZENE

Dinitrobutyl fluoroxylene.
A Nitromusk related to Musk Ketone
(Acetyl- instead of Fluoro-).



$C_{12}H_{15}FN_2O_4 = 270.27$

Pale yellowish crystals. M.P. 64° C.

Insoluble in water, poorly soluble in alcohol, fairly soluble in most oils, but poorly in hydrocarbons (Terpenes, etc.).

This "Halogen"-musk was developed mainly for the purpose of investigating the effect of the various Halogen atoms upon the musk type odor. It was confirmed that the lower the Halogen atomic weight, the lower the melting point (and the higher the evaporation) of the Nitromusk.

However, the physical effect of evaporation rate is not strictly parallel to the fixative effect or the desired musk effect. Although it can be said that the title musk has an initially stronger odor than Musk Ketone, its odor type is less desirable and its tenacity poorer.

The hazard of having Fluorine in a molecule, no matter where it is attached, will generally scare perfumers or chemists from using such chemical in perfumes or cosmetic preparations.

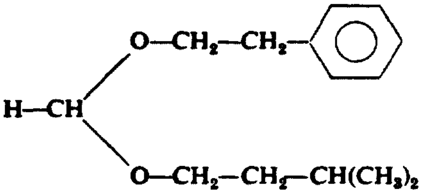
The title material is included as an example of these rarer types of Nitromusk. It may be considered as practically obsolete.

Prod.: basically from *tertiary*-Butyl xylene, or even from *meta*-Xylene. The title musk is obtained by fluorination instead of Acetylation.

95-197; 96-230;
see also: 31-196;

## 1393: FORMALDEHYDE-iso-AMYL PHENYLETHYL ACETAL

A "mixed" acetal, related to several known specialties.



$C_{14}H_{22}O_2 = 222.33$

Colorless oily liquid. B.P. 249° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, sweet-green, slightly floral, rosy odor of considerable tenacity. However, the overall character is not very distinct, since it seems to have notes from Rose, Hyacinth, etc. blended with winey-weedy tonalities in an overall odor impression that leaves the observer somewhat confused.

This acetal is a member of a very long series of acetals prepared in search of interesting green-floral, soap-stable chemicals. Many were found and are still in use, but the newer chemicals (e. g. the Hexenol-series) have more power and distinction.

This acetal could find use in Rose, Hyacinth, Appleblossom, etc. as well as in various types of Oriental fragrances. It may lend part of the desirable "natural" greenness, accompanied by a certain amount of sweet floral notes.

Prod.: from Formaldehyde-di-*iso*-Amyl-acetal plus Phenylethyl alcohol – usually by short-time boiling.

5-321;

## 1394: FORMALDEHYDE-DI-iso-AMYLACETAL

Di-*iso*-amyl methylal.

$H—CH(O—CH_2—CH_2—CH(CH_3)_2)_2$

$C_{11}H_{24}O_2 = 188.31$

Colorless liquid. Sp.Gr. 0.88. B.P. 110° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet, but faint, slightly fruity, Pear-like odor, remotely reminiscent of Terpinyl acetate or Linalyl acetate, sweeter than the former, not as sweet as the latter.

This acetal has been suggested for use in perfume compositions to assist in bringing Citrusy (particularly Bergamot-like) topnotes out and to give impression of sweet freshness.

The effect of this acetal is, however, not very powerful, and not as pleasant as one could wish for above purpose.

Prod.: from Formaldehyde and *iso*-Amyl-alcohol. In place of Formaldehyde its dimethyl acetal may be used in the condensation.

31-72; 37-281; 86-53;

## 1395: FORMALDEHYDE DIBUTYL ACETAL

Dibutyl formal.
Methylene dibutylether.

$H—CH(O—C_4H_9)_2$

$C_9H_{20}O_2 = 160.26$

Colorless mobile liquid. B.P. 85° C.
Sp.Gr. 0.83.

Very slightly soluble in water, soluble in alcohol and oils.

Ethereal-fruity odor, reminiscent of Butyl formate and Dibutyl ether.

Has been suggested for use in flavor compositions – mostly in fruit complexes, where it may introduce an ethereal lift in imitation Strawberry and Raspberry, perhaps in Pineapple, etc.

The subject acetal is NOT listed in the G.R.A.S. list of the American Federal Register, but the material may be used in food flavors in certain countries.

Prod.: from Chloromethyl methylether and Sodium butoxide.

37-281; 86-53;

## 1396: FORMALDEHYDE DIETHYLACETAL

Diethyl methylal.
Methylene diethylether.
Diethyl formal.

H—CH(O—$C_2H_5$)$_2$

$C_5H_{12}O_2 = 104.15$

Colorless mobile liquid. Sp.Gr. 0.85.
B.P. 87° C.

Miscible with water, alcohol and oils.

Very diffusive, sweet-ethereal odor, somewhat reminiscent of Acetone and Methyl acetate.

Sweet, ethereal, slightly fruity taste. Not very powerful.

This acetal finds perhaps a little use in perfume compositions where its exceptional diffusive power can augment the radiation of certain types of topnote, e. g. Citrusy, winey or green topnotes.

However, it causes considerable problems to hold back the evaporation of this acetal in a perfume, and it tends to "override" the entire topnote within the first few seconds, unless it is exceptionally well fixed.

Prod.: from Chloromethyl methylether plus Sodium ethoxide.

37-281; 66-482; 86-53;

## 1397: FORMALDEHYDE DIMETHYLACETAL

Methylal.
Formal.
Methylene dimethylether.
Dimethoxy methane.

H—CH(OCH$_3$)$_2$

$C_3H_8O_2 = 76.10$

Colorless mobile liquid. Sp.Gr. 0.87.
B.P. 42° C.

33 % soluble in water, miscible with alcohol, soluble in some oils, not in all.

This acetal which, to the author's knowledge, is not used as such in perfumes or flavors, is mentioned because it is not only a good solvent and used for that purpose in extractions, but it is also an intermediate in making other acetals from Formaldehyde. It is therefore often a trace component-impurity in the lower alifatic acetals, and should be recognized as such.

It has an extremely diffusive, ethereal odor, resembling that of Methyl formate or Ethyl nitrite, briefly: ethereal.

Prod.: from Chloromethyl methylether plus Sodium methoxide.

26-614; 31-72; 37-281; 66-482; B-I-574;

## 1398: FORMALDEHYDE DIPROPYL ACETAL

Dipropyl formal.
Methylene dipropylether.

H—CH(O—$C_3H_7$)$_2$

$C_7H_{16}O_2 = 132.21$

Colorless mobile liquid. B.P. 68° C.
Sp.Gr. 0.81.

Slightly soluble in water, soluble in alcohol and in most oils.

Very diffusive, ethereal odor, reminiscent of Dipropyl ether and Propyl formate.

Has been suggested for use in perfumes and flavors, but its very low boiling point causes considerable problems for its use in perfumes, except perhaps in a few cases where an ethereal topnote resembling that of "aged" alcohol is desirable.

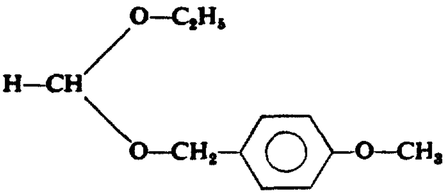
Its flavor does not describe any fruit, it is simply ethereal and rather weak, yet quite sweet.

Prod.: from Chloromethyl methylether plus Sodium propoxide.

37-281; 66-482; 86-53;

## 1399: FORMALDEHYDE ETHYL ANISYL ACETAL

A "mixed" acetal.



$C_{11}H_{16}O_3 = 196.25$

Colorless oily liquid. B.P. 252° C.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet-floral and very tenacious odor.

Sweet, floral, slightly winey-Vanilla-like taste.

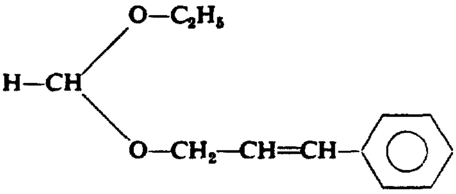
This acetal was probably marketed because it was considered an improvement over Anis-alcohol from an olfactory point of view. However, it does not have much more power, and not the versatile floral character as found in Anis alcohol.

Prod.: from Formaldehyde diethylacetal plus Anisalcohol.

5-321;

## 1400: FORMALDEHYDE ETHYL CINNAMYL ACETAL

A "mixed" acetal.



$C_{12}H_{16}O_2 = 192.26$

Colorless, slightly viscous liquid.
B.P. 264° C.

Insoluble in water, soluble in alcohol and oils.

Very sweet, floral-balsamic, warm, yet refreshingly clean odor.

This chemical, which is rarely offered under its proper chemical name, but is marketed as a major part of several specialties, known for decades, has some advantage over Cinnamic alcohol, other than its fresher, greener odor: it seems to be less susceptible to oxidation than Cinnamic alcohol, in which an undesirable odor of Cinnamic aldehyde often appears after short time storage.

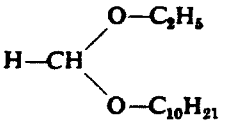
It could find use as a major ingredient in floral bases, Hyacinth, Appleblossom, Lilac, etc., as well as in Oriental fragrance types. It blends well with Sandalwood and the Ionones, with Phenylpropylalcohol or Phenylethyl propionate for the attractive "fruity-green" notes, etc.

Prod.: from Formaldehyde diethylacetal plus Cinnamic alcohol by short-time boiling.

5-321;

## 1401: FORMALDEHYDE ETHYL DIMETHYLOCTANYL ACETAL

A "mixed" acetal.



(Structure – see Dimethyl octanol).

$C_{13}H_{28}O_2 = 216.37$

Colorless oily liquid. B.P. 231° C.

Insoluble in water, soluble in alcohol and oils.

Green, waxy-rosy, sweet, overall floral odor of moderate tenacity.

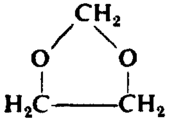
Although the odor of this acetal is somewhat different from that of the parent fragrant alcohol, it has so little extra to offer that it is most conceivable that the material will never become a standard perfume ingredient. The green notes can be achieved in greater variety with other materials, and the rosy notes are actually weaker than those of the Dimethyl octanol itself.

Prod.: from Formaldehyde diethylacetal plus Dimethyl octanol by short-time boiling.

5-321;

## 1402: FORMALDEHYDE ETHYLENEGLYCOL ACETAL

Dioxolane.
Dioxolan.
Glycol methylal.
*1,3*-Dioxolan.
Glycol formal.
Glycol methylene ether.



$C_3H_6O_2 = 74.08$

Colorless mobile liquid. B.P. 76° C.
Sp.Gr. 1.06.

Miscible with water, alcohol and most oils.

Very diffusive, slightly choking or nauseating, Pear-like odor of very poor tenacity. In aqueous dilution the odor appears very weak mainly due to the miscibility of the acetal with water.

The taste is sweet, mildly ethereal-fruity.

The subject acetal is mentioned in this work mainly because it is an important parent or prototype of a group of interesting perfume and flavor chemicals, and related to the Dioxanes.

The title material is also used as a solvent in the extraction of flavors from natural raw materials.

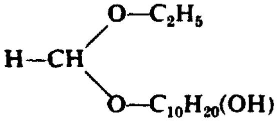
A great number of acetals, formed with Ethyleneglycol, have become useful perfume or flavor materials, and homologues are prepared from Propylene glycol or other glycols.

Prod.: by condensation of Formaldehyde with Ethylene glycol.

26-564; 31-72; B-XIX-2;
see also: Dioxan (Dioxane).

## 1403: FORMALDEHYDE ETHYL HYDROXYCITRONELLYL ACETAL

Not a well defined, single chemical.
A mixed acetal, mainly:



$C_{13}H_{28}O_3 = 232.37$

Colorless viscous oil. B.P. 268° C.

Insoluble in water, soluble in alcohol and oils.

Very mild, refreshing, green-floral, Citrus-like, Lemon-type odor of good tenacity.

Many attemps have been made to develop materials with the olfactory properties of Hydroxycitronellal and with none of its drawbacks, such as those arising from the aldehyde group.

The equivalent alcohol, Hydroxycitronellol, has been suggested as a stabilizer for the aldehyde, but the alcohol has very little odor. The acetals of Hydroxycitronellal have, when pure, very little odor value.

The subject "mixed" acetal was developed with similar thoughts in mind. But it does not have the floral richness of Hydroxycitronellal, and its additional lemony notes are certainly not desirable in the fragrances where the aldehyde is normally applied.

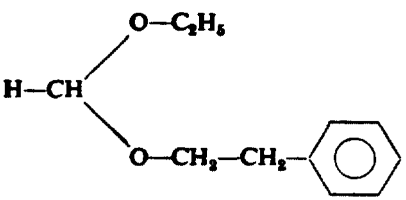
This acetal remains therefore, largely a curiosity, rather than a standard shelf item in the perfume laboratory.

Prod.: from Formaldehyde diethyl acetal plus Hydroxycitronellol by short-time boiling.

5-321;

## 1404: FORMALDEHYDE ETHYL PHENYLETHYL ACETAL

A "mixed" acetal.



$C_{11}H_{16}O_2 = 180.25$

Colorless oily liquid. B.P. 226° C.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet, rosy-green odor of moderate tenacity.

As a variation of the Phenylethyl alcohol/Phenethylethyl acetate/Phenylacetaldehyde-dimethylacetal-theme, the subject acetal has some merit for its refreshingly rosy notes. However, it lacks power and is not more tenacious than the Phenylethyl alcohol itself.

It could find some use in Rose, Hyacinth, and in various herbaceous fragrance types, where the sweet-green notes could be utilized in the topnote composition.

Prod.: from Formaldehyde diethylacetal plus Phenylethyl alcohol by short-time boiling.

5-321;

## 1405: FORMALDEHYDE ETHYL »RHODINYL« ACETAL

Not a well defined single chemical.

The few commercial products ever marketed were presumably prepared from Rhodinol, isolated from Geranium oil by saponification and fractional distillation (see monograph: Rhodinol). Other products under this name may have been prepared with *laevo*-Citronellol, or simply with ordinary Citronellol.

It serves little purpose to make an odor description of a product which is rarely offered, and hardly in a standard grade or composition.

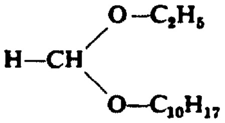
It was developed to produce a perfume chemical with the virtues of Rhodinol plus a refreshing greenness, a combination ideal for Muguet bases.

Prod.: from Formaldehyde diethylacetal plus "Rhodinol" by short-time boiling.

5-321;

## 1406: FORMALDEHYDE ETHYL TERPINYL ACETAL

A "mixed" acetal, but not a well-defined, single chemical.
Structure of main component – see also Terpineol.



$C_{13}H_{24}O_2 = 212.34$

Colorless oily liquid. Insoluble in water, soluble in alcohol and perfume oils.

Herbaceous, sweet-green and slightly fruity-ethereal odor of moderate tenacity.

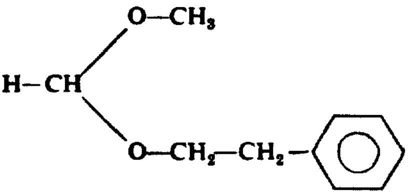
Suggested for use in fragrance compositions, but does not seem to offer any advantage over Terpinyl acetate plus "sweet-herbaceous-green" chemicals. Various experimental batches have been sampled to the industry, and the odor varies considerably according to the method of production and according to the type of Terpineol used in the reaction.

Prod.: from Formaldehyde diethylacetal plus Terpineol by short-time heating.

5-321;

## 1407: FORMALDEHYDE METHYL PHENYLETHYL ACETAL

A "mixed" acetal.



$C_{10}H_{14}O_2 = 166.22$

Colorless oily liquid. Very slightly soluble in water, soluble in alcohol and perfume oils.

Ethereal-green, yet sweet and slightly floral-rosy odor of poor tenacity. The greennes resembles that of foliage mixed with flowers, but it is somewhat "gassy" ethereal, not quite pleasant.

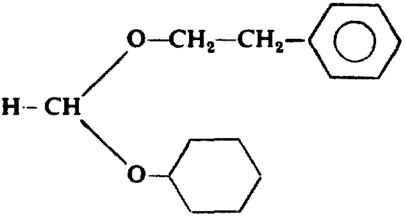
Has been suggested for use in floral and non-floral fragrances to assist in producing true-to-Nature green foliage notes. However, the acetals from Acetaldehyde are superior from an odor point of view, normally free from the overly diffusive or "gassy" notes.

Prod.: from Formaldehyde dimethylacetal plus Phenylethyl alcohol by short-time boiling.

5-321;

## 1408: FORMALDEHYDE PHENYLETHYL CYCLOHEXYL ACETAL

A "mixed" acetal.



$C_{15}H_{22}O_2 = 234.34$

Colorless, somewhat viscous liquid.
B.P. 276° C.

Insoluble in water, soluble in alcohol and oils.

Somewhat musty-woody, faintly musky odor with rosy undertones. The "musky" character is not exceptionally pleasant, and the term "musky" is, in fact, often applied to materials, the odor of which is hard to describe because the odor level is low (compare Benzyl salicylate, Farnesol, etc.).

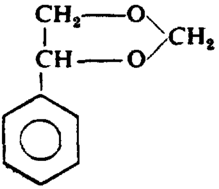
The author feels that this material is of little or no interest to the perfumer beyond that of the academic interest.

Prod.: from Formaldehyde di-phenylethyl acetal plus Cyclohexanol by heating.

5-321;

## 1409: FORMALDEHYDE PHENYLETHYLENEGLYCOL ACETAL

*4*-Phenyl-*1,3*-dioxacyclopentane.
Phenylglycol methylene ether.
Phenylglycol methylacetal (confusing name).
(Phenylglycol methylene acetal).
"Jasmal" (old Verley name).
*4*-Phenyl-*meta*-dioxolan.
This cyclic acetal is also part of
several well-known perfume specialties.



$C_9H_{10}O_2 = 150.18$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol and perfume oils.

Peculiar oily-herbaceous odor, not unlike that of Amylcinnamic aldehyde, but not as tenacious, not as purely oily-herbaceous. The subject acetal has a more musty note, quite typical of many glycol acetals.

In actual use, however, almost floral notes are brought about, again an effect resembling that of A.C.A. The odor is overall mild, and the material can be applied at rather high concentration.

Its odor remains inferior to many modern and even some old, well-established fragrance materials for Jasmin notes, and it is doubtful whether this acetal will ever become commonly used.

Prod.: from Phenylethylene glycol and Formaldehyde with water and Sulfuric acid, by heating.

5-322; 31-72; 103-285; 86-115;
See also: Phenylacetaldehyde ethyleneglycolacetal.

## 1410: FORMIC ACID

Methanoic acid.

H—COOH

$CH_2O_2 = 46.03$

Colorless mobile liquid. Sp.Gr. 1.22.
B.P. 101° C.
Solidifies in the cold, melts at 8° C.

Miscible with water, alcohol, Propylene glycol, Glycerin, perfume and flavor oils.

Pungent odor giving a stinging sensation on the mocous membranes. Sour taste in proper dilution – lower than 50 ppm without stinging or burning.

Corrosive and harmful to human skin and mucous membranes unless diluted.

This acid finds use in flavors, usually NOT incorporated in the flavor composition because of its high acidity which is a threat to the esters and alcohols in a flavor, but it is used as a separate additive to the functional, final consumer product.

It is also used as a preservative in certain countries.

In the less common cases where the acid *is* used in the flavor composition itself, it may enter at concentration equal to 1 to 20 ppm in the finished product.

As a food preservative, it may be used at 500 to 2500 ppm in concentrated fruit juices, etc. intended for dilution prior to consumption. In certain countries, the acid is incorporated only in the unsweetened juices, and the acid is therefore virtually removed from the consumer product when sugar is added and the syrup brought to boiling point in the final processing.

Formic acid is particularly adaptable to the flavor of Pineapple.

The esters of Formic acid (Formates) are known for their sweetness of flavor (lower alifatic esters) and powerful green-herbaceous character (certain aromatic formates).

Prod.: from Carbon monoxide by treatment under heat and pressure with water or with Sodium hydroxide solution. The latter method produces the Sodium salt of Formic acid.

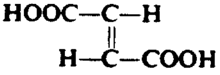
G.R.A.S. F.E.M.A. No.2487.

26-556; 66-540; 77-178; 77-212; 77-268; 100-461; 160-1000; B.II.8; 140-131;

## 1411: FUMARIC ACID

*trans-alpha-beta*-Ethylene-*1,2*-dicarboxylic acid.
Allo-maleic acid.
*para*-Maleic acid.
*trans*-Butene dioic acid.
Boletic acid.

(The *cis*-isomer is Maleic acid).



$$\begin{array}{l} HOOC-C-H \\ \quad\quad\quad\;\, \| \\ \quad\;\; H-C-COOH \end{array}$$

$C_4H_4O_4 = 116.08$

White or colorless prismatic, needlelike or leafy crystals. M.P. approximately 288° C. (decomposes under open melting).

The acid will sublime when heated to melting point.

0.5% soluble in water, 6% soluble in cold alcohol, 10% soluble in boiling hot water, 5% in hot alcohol. Poorly soluble in oils.

Virtually odorless. Clean, slightly tart, acid taste in aqueous solution.

This acid is used in food products as an acidifier with an acid type of taste that blends particularly well with caramellic or sugar-sweetened products, baked products, etc.

The drawback of slow solubility in water is greatly overcome by the addition of 0.3% of a wetting agent to the Fumaric acid. One commercial product CWS Fumaric acid (cold water soluble) contains 0.3% Dioctyl sodium sulfosuccinate (Monsanto) and dissolves quickly in ice cold water.

It is also used along with imitation Apple flavor, Peach and Vanilla.

A special use is that in baking powders, partly or wholly as a substitute for Tartaric acid (decomposition under heating produces harmless gases in the baking process).

The concentration used is equivalent to 50 ppm in beverages, and up to 3600 ppm in gelatin desserts.

Prod.: (many methods) e. g. by fungal action upon Glucose.

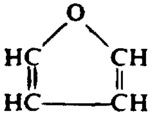
2) by isomerization of Maleic acid.
3) by oxidation of Furfural with Sodium chlorate and catalyst.

G.R.A.S. F.E.M.A. No.2488.

66-989; 26-556; 100-465; 160-1004; B-II-737; 140-146;

## 1412: FURAN

Furfuran.
Divinylene oxide.
Tetrole.
Oxole.



$C_4H_4O = 68.08$

Colorless liquid. Sp.Gr. 0.94. B.P. 32° C.

0.8% soluble in water, soluble in alcohol and oils.

Resinifies easily, e. g. when evaporated in the open.

Peculiar spicy-smokey, slightly Cinnamon-like odor.

This oxide is occasionally used in the composing of artificial essential oils. It finds a little – rare – use in industrial fragrances for certain masking purposes, e. g. when the problem is: to mask very volatile, undesirable odors.

Occasionally, this item is used in special fragrances such as "smokey" odors for certain products, directly or indirectly connected with food products.

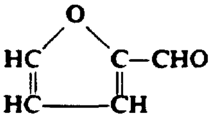
Prod.: by decarboxylation of Furoic acid.

Furan can also be prepared directly from Furfural.

4-53; 26-558; 31-150; 69-144; 85-63; 86-53; 100-466; 160-1004; B-XVII-27;

# 1413: FURFURAL

*alpha*-Furyl formaldehyde.
*2*-Formylfuran.
*2'*-Oxo-*2*-methylfuran.
Furan-*2*-aldehyde.
Pyromucic aldehyde.
Furan-*alpha*-aldehyde.
"Furfurol" (misleading name).
"Furol" (misleading name).
*2*-Furaldehyde.
*2*-Furancarbonal.
Fural.
Furfuraldehyde.



$C_5H_4O_2 = 96.09$

Colorless liquid which turns amber-colored, then dark brown when exposed to air and daylight. Sp.Gr. 1.16. B.P. 162° C. Flammable liquid.

Soluble 9% in cold water, 20% in hot water. Soluble in alcohol and most perfume and flavor oils, but not in hydrocarbons (Terpenes, etc.).

Pungent, but sweet, bread-like, caramellic, Cinnamon-Almond-like odor of poor tenacity.

Sweet, bread-like, caramellic taste in proper dilution.

This aldehyde finds a little use in perfumery, mostly as a trace component in artificial essential oils and flower absolutes.

It is widely used in flavor compositions for imitation Butter, Butterscotch, Caramel, Coffee, Bread, Molasses, Fruit, Nut, Cinnamon (Cassia), Brandy, Rum, Rye, etc.

The concentration used is about 1 to 30 ppm in the finished product.

Prod.: by hydrolysis, followed by dehydration of Pentosane-rich plant material, such as Corn cobs, Peanut shells, Oat hulls, etc.

G.R.A.S.*) F.E.M.A. No.2489.

Furfural is an extremely interesting flavor material, not only in itself, but it serves as starting material for the manufacture of a very great number of important perfume and flavor materials, many of quite recent date of development. It forms substituted aldehydes by condensation with alifatic aldehydes, similar to the process used in making Amylcinnamic aldehyde from Benzaldehyde, and it will condense with ketones to form other aroma chemicals. The corresponding acid and alcohol further serve as stepping stones in making other aroma chemicals.

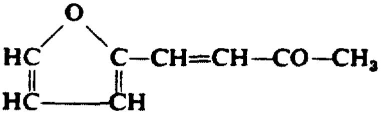
4-53; 26-556; 69-152; 77-208; 85-63; 90-796; 100-466; 160-1006; B-XVII-272; 140-173;

*) Although tolerated in quantities of several grams per day per adult person, Furfural can cause severe headache after single doses of 0.06 grams, inhaled or ingested.

# 1414: FURFURAL ACETONE

*2*-Furylidene acetone.
Furfurylidene acetone.
*4*-(*2*-Furyl)-*3*-buten-*2*-one.
"Furfuryl acetone".

**Note**: The perfume and flavor literature shows great confusion with respect to the nomenclature of substituted Furfurals.



$C_8H_8O_2 = 136.15$

Colorless, needle-like crystals. M.P. 40° C. B.P. 229° C. (decomposes).

Insoluble in water, soluble in alcohol and most oils.

Mild, warm, spicy-woody, sweet odor, somewhat reminiscent of Cinnamon.

Sweet, warm, slightly Cinnamon-like taste.

This ketone finds a little use in flavor compositions, not only for imitation Cinnamon -and Cassia), but also for Nut flavor and Grape.

It is rarely, if ever, used in perfumes.

The concentration used in flavors is equivalent to about 2 to 50 ppm in the finished product.

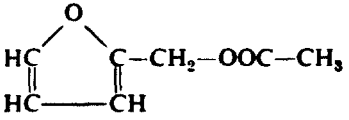
Prod.: by condensation of Furfural with Acetone.

G.R.A.S. F.E.M.A. No.2495.

26-558; 69-155; 77-212; 86-53; 160-778; B-XVII-306; 140-174;

## 1415: FURFURYL ACETATE

*2*-Furyl carbinyl acetate.



$C_7H_8O_3 = 140.14$

Colorless oily liquid. Sp.Gr. 1.12.
B.P. 176° C.

Insoluble in water, soluble in alcohol and oils.

Mild, ethereal-floral odor, somewhat reminiscent of Ethyl acetoacetate, Benzyl acetate and the Glycol acetates, with a herbal-spicy undertone.

Pleasant, warm-fruity, partly herbaceous and rather nondescript taste. Not reminiscent of any particular, natural product, nevertheless overall pleasant. In high concentration it shows a "bite" or a herbaceous pungency.

The ester finds, to the author's knowledge, little or no application in perfumery.

It is used in flavor compositions for imitation Raspberry and in fruit complexes, spice blends, e. g. in "Ginger Ale" types, etc.

The concentration used is about 1 to 40 ppm in various food products, and as high as 500 ppm in chewing gum.

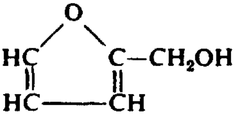
G.R.A.S. F.E.M.A. No.2490.

Prod.: from Furfural by hydrogenation to Furfuryl alcohol. Acetylation yields the acetate.

26-558; 31-127; 43-500; 69-151; 86-53; 160-1006; B-XVII-112; 140-173;

## 1416: FURFURYL ALCOHOL

*alpha*-Furyl carbinol.
*2*-Furyl carbinol.
Furfuralcohol.
*2*-Hydroxymethyl furan.



$C_5H_6O_2 = 98.10$

Colorless or pale yellowish, slightly oily liquid. Sp.Gr. 1.13. B.P. 171° C.

Miscible with water and alcohol, soluble in many flavor oils, but not in hydrocarbons (e. g. Terpenes).

Resinifies easily, particularly under acid conditions. Decomposes slowly in aqueous solution.

Very mild, warm-oily, "burnt" odor. Chemically pure Furfuryl alcohol is – in the opinion of many observers – virtually odorless.

Warm, slightly caramellic taste, in higher concentration burning, yet somewhat creamy.

Occasionally used as a solvent in perfumery or in certain cosmetic preparations.

Used in flavor compositions for imitation Coffee, Butter, Butterscotch, Caramel, in fruit complexes, Brandy flavors, etc.

It is a natural component (about 50 %) of the volatile oil from Coffee bean meal (of roasted Coffee).

Concentration used is equivalent to about 10 to 100 ppm in the finished product.

Prod.: by hydrogenation of Furfural.

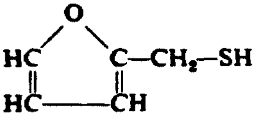
The production from Coffee bean meal is of less economic interest.

G.R.A.S. F.E.M.A. No.2491.

7-136; 69-151; 90-769; 100-467; 160-1006; B-XVII-112; 140-173;

## 1417: alpha-FURFURYL MERCAPTAN

*2*-Furan methane thiol.
*2*-Furyl methane thiol.



$C_5H_6OS = 114.17$

Colorless oily liquid. Sp.Gr. 1.13.
B.P. 155° C.

Insoluble in water, soluble in alcohol and oils.

Extremely powerful and diffusive, penetrating odor, only in proper dilution being agreeable, Coffee-like, caramellic-burnt, sweet.

Although not the most powerful odorant known, Furfuryl mercaptan is one of the most powerful and penetrating odors used in flavors. It has always amused statisticians to calculate that it might not take more than 10 (ten) grams of Furfuryl mercaptan to perfume enough air so that every human being on earth could smell it.

Dilutions below 5 ppm have a pronounced caramellic-Coffee-like taste and odor.

This material is used in flavor compositions, mainly imitation Coffee, also "reconstituted instant Coffee", and in Chocolate flavors, fruit and Nut complexes, Treacle caramel, etc.

The concentration used is about 0.1 to 2 ppm in the finished product. It is highest in hard candy or other heat-processed candy.

Prod.: from Furfuryl alcohol plus Hydrogen sulfide to make Difurfuryl disulfide, which is reduced to the Mercaptan.

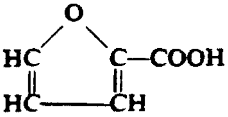
G.R.A.S. F.E.M.A. No.2493.

4-53; 26-558; 69-151; 30-22; 160-1008; 85-64; 159-28;

Readers who are interested in a detailed report on volatile components in Coffee, should consult M.A.Gianturco's chapter of book No. 157. (See literature index).

## 1418: 2-FUROIC ACID

Furan-*2*-carboxylic acid.
Furan-*alpha*-carboxylic acid.
Pyromucic acid.



$C_5H_4O_3 = 112.09$

White crystal needles. M.P. 133° C.
B.P. 232° C. (sublimes before melting).

3.6% soluble in water, soluble in alcohol, miscible with oils.

Practically odorless.

Clean acid taste with a mildly caramellic note.

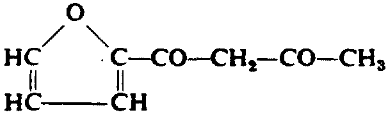
Although this acid is rarely used as such in flavors, it serves as an intermediate in the preparation of a great number of interesting flavor chemicals, and thus participates indirectly in artificial flavorings.

Prod.: from Furfural by oxidation or by Canizzaro reaction (dismutation of Furfural by alkali reaction to yield the acid and the alcohol).

26-558; 69-157; 100-467; 160-1008; B-XVIII-272;

## 1419: FUROYL ACETONE

Pyromucyl acetone.
*1*-(*2'*-Furyl-)-*1,3*-butandione.



$C_8H_8O_3 = 152.15$

Yellowish crystalline mass.

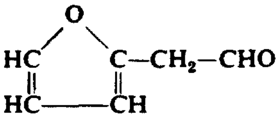
Sweet, buttery-cinnamon-like odor of moderate tenacity, but quite penetrating.

This ketone has been suggested for use in perfumes for its powerful, warm-spicy character and sweetness, but it is most likely that fear of irritating effect has prevented more wide use of this chemical.

Prod.: from *2*-Acetyl furan by reaction with Ethyl acetate and Sodium ethoxide. It has also been produced from Ethyl furoate and Acetone by condensation with Sodamide.

## 1420: 2-FURYL ACETALDEHYDE

Furanacetaldehyde.



$C_6H_6O_2 = 110.11$

Colorless or pale yellowish liquid.

B.P. 156° C.

Almost insoluble in water, soluble in alcohol and oils.

Rather sharp, but warm, green-spicy, pungent odor.

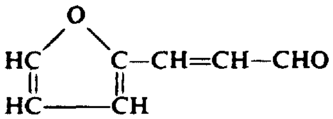
This material has been suggested for use in floral perfume types as a powerful floral-green note, not as sharp as Phenylacetaldehyde. However, this aldehyde is not very stable, and is probably more or less abandoned in perfumery of today.

Prod.: from Furfural plus Methyl monochloro acetate to make the glycidic ester. Subsequent hydrolysis yields the aldehyde.

69-154;.

## 1421: FURYL ACROLEIN

*beta-2*-Furyl acraldehyde.
*2*-Furan acrolein.
*beta-2*-Furyl propenal.
Furacrolein.
"Furfur acrolein" (misleading name).



$C_7H_6O_2 = 122.13$

Yellowish or amber-colored crystals.

M.P. 54° C. B.P. 220° C. Sp.Gr. 1.12 (liquid).

Insoluble in water, miscible with alcohol and oils.

Warm, sweet, woody-cinnamon-like odor, remotely reminiscent of Coffee.

Sweet, warm-spicy taste, reminiscent of Cinnamon.

This aldehyde is, to the author's knowledge, not used in perfumery, perhaps because of its tendency to discolor.

It finds use in flavor compositions, mainly for imitation Coffee and Cinnamon, also for fruit complexes, Rum variations, Caramel, etc.

Concentration used vary from as little as 0.1 ppm to 40 ppm in the finished product. Its relatively low vapor pressure – as compared to Cinnamic aldehyde – makes it somewhat preferred in baked goods and flavors for other heat processed goods.

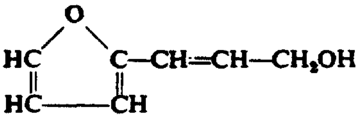
G.R.A.S. F.E.M.A. No.2494.

Prod.: from Furfural and Acetaldehyde by condensation.

31-40; 69-154; 160-786; 93-150; 95-148;

## 1422: 2-FURYL ALLYLALCOHOL

*beta*-Furyl allylalcohol.



$C_7H_8O_2 = 124.14$

Colorless oily liquid. Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet and warm-herbaceous, also caramellic-balsamic odor of moderate to poor tenacity.

The author is not aware of any application of this alcohol in perfume compositions. It may find limited use as a trace component in certain artificial essential oils and flower absolutes.

This alcohol has been suggested for use in flavor compositions for its natural, sweet and warm-mellowing effect in imitation Brandy, Wine, Rum, etc. and in Caramel or Nut compositions, Cherry and a few other fruity types, etc.

The concentration used is normally equivalent to 20 to 50 ppm in the finished product.

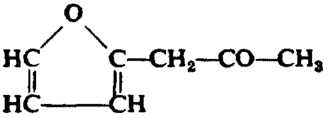
The title material is *not* mentioned in the Federal Register or listed by the F.E.M.A. as "G.R.A.S." and it should therefore be considered as banned from use in food flavors in the U.S.A.

Prod.: e. g. from Furfural by condensation with Acetaldehyde, followed by reduction of the *beta-2*-Furylacraldehyde.

(See also: 69-151 and 69-154).

## 1423: (2-FURYL)-2-PROPANONE

Furyl acetone.
(Do not confuse with Furoyl acetone).



$C_7H_8O_2 = 124.14$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet, fruity-caramellic, somewhat spicy odor.

Sweet, fruity-spicy, slightly Nut-like taste.

This ketone is used in flavor compositions, mainly fruity types, also combination flavors for ice cream, etc.

Concentration used is normally about 2 to 20 ppm in the finished product.

Prod.: from *2*-Methylfuran plus Acetyl chloride.

G.R.A.S. F.E.M.A. No.2496.

## 1424: FUSEL OIL

See also monograph: Amyl alcohol.

Fusel oil is not a well-defined chemical, but it is mentioned in this work because it is used in flavors and it serves as an intermediate in the preparation of a great number of flavor chemicals, all having the special character of Fusel oil if they were prepared from that material rather than from synthetic Amyl alcohol.

Fusel oil is made by distillation of the "pot residue" after distillation of Rum or other sugar- or starch-fermented alcoholic distilled beverages. It contains decomposition products of the plant proteins remaining in the fermentation liquid from which the alcohol was distilled.

There are many types of fusel oil:

1) from grain (mainly in the U.S.A.)
2) from molasses of sugar cane (mainly in the West Indies)

3) from molasses of sugar beets (mainly in Scandinavia)
4) from potato (mainly in Scandinavia and Germany)
5) from Rice (mainly Indonesia and Japan)
6) from Grape (wine distillation) (mainly France).

Fusel oil varies in composition according to the origin. It is conventionally valued after its content af "Amyl alcohols" which may be as low as 50% or as high as 90%.

The chief components are:

1) *2*-Methylbutanol-*1*. (an *iso*-Amyl alcohol)
2) *2*-Methylbutanol-*4*. (an *iso*-Amyl alcohol)
3) *iso*-Butyl alcohol.
4) Propyl alcohol
5) Ethyl alcohol
6) Capric acid (Decanoic acid) and esters
7) traces of Furfural, Diacetyl, Acetaldehyde and other Aldehydes and Ketones, etc.

Fusel oil is usually a colorless oily liquid, slightly soluble in water, miscible with alcohol and most oils.

Vinous-ethereal, at times pungent, sometimes mild, oily smelling with considerable variations according to origin.

It is used in certain artificial essential oils.

Fusel oil finds use in flavor compositions, mainly in imitation Wine, Cognac, Liqueur, Brandy, Rum, Arak, etc.

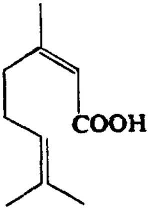
The concentration used may vary from 2 to 30 ppm in the finished product, but can be as high as 300 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2497.

31-16; 77-170; 77-182; 140-123;

## 1425: GERANIC ACID

*3,7*-Dimethyl-*2,6* (and *2,7*)-octadienoic acid.
The commercial product is a mixture of *cis*- and *trans*-isomers.



$C_{10}H_{16}O_2 = 168.24$

Colorless liquid, slightly viscous, and increasing in viscosity with age or exposure to air and daylight.
Sp.Gr. 0.97. B.P. 250° C. (approximately).

Insoluble in water, soluble in alcohol and oils.

Mild, green-floral, also slightly weedy, but overall fresh and clean odor with woody undertones. It bears some resemblance to the odor of Geraniol tail fractions.

This acid, only recently marketed on a commercial scale, has been suggested for use in imitation Geranium oil and in other artificial essential oils. It is particularly interesting in assisting the peculiar undertones in Clary Sage oil (artificial). In general, it introduces a certain amount of "lasting lift" to a fragrance, and it blends with floral as well as with non-floral types, although it is much easier to apply to the herbaceous and woody types.

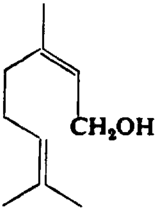
Prod.:

1) from *2*-Methylhepten-*2*-one-*6* with Iodo- or Bromoacetic ester and a Zinc type catalyst.
2) by oxidation of Citral.

6-144; 66-645; 90-134; 160-1010;

## 1426: GERANIOL

*2-trans-3,7*-Dimethyl-*2,6*-octadien-*8*-ol.
"Meranol" (A. Boake, Roberts & Co.).



$C_{10}H_{18}O = 154.26$

Colorless oily liquid. May turn pale yellowish (and change odor) by absorbing oxygen from air. Sp.Gr. 0.89. B.P. 230° C.

Slightly soluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Mild and sweet, floral Rose-type odor. Warm and yet slightly dry undertones, but there are great variations according to the quality and origin of the Geraniol.

One of the most frequently used perfume chemicals, this alcohol finds its way into all types of perfumes for all kinds of purposes, from delicate lotion perfumes and soft cosmetic fragrances to sweet floral household odors and even the least expensive soap perfumes.

Although primarily a rose material, Geraniol is used generally as a sweet floral material of outstanding versatility. It forms conventionally a major part of most artificial YlangYlang bases, and is often included in creations of Peony, Sweet Pea, Frangipanni, Magnolia, etc. etc.

Its taste is somewhat disappointing, somewhat bitter unless used at very low concentration. Nerol is generally preferred for better sweetness. However, Geraniol finds its way into multitude of flavor types, such as Apple, Apricot, Strawberry, Raspberry, Plum, Peach, Honey, Cherry, Lemon, Cassia, Cinnamon, Nutmeg, Rootbeer, Ginger Ale, etc.

Concentrations are usually kept as low as 1 to 10 ppm in the finished product, more because of the lack of sweetness than because of any fear of toxicity.

Prod.:

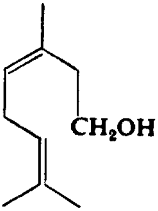
1) by isolation from Palmarosa oil or from Citronella oil.
2) by reduction of Citral a.
3) from Pinene via Myrcene and its Hydrochloride to Geranyl chloride.

G.R.A.S. F.E.M.A. No.2507.

4-54; 5-16; 26-518; 77-173; 85-64; 86-54; 87-539; 103-224; 106-168; 156-166; 160-1010; B-I-457; 140-126;

## 1427: iso-GERANIOL

*3,7*-Dimethyl-*3,6*-octadienol.



$C_{10}H_{18}O = 154.26$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Sweet-rosy odor, not as mild as Geraniol, and not as fruity, more herbaceous or remotely green, less "creamy".

Floral, but not quite sweet taste, overall weaker than that of Geraniol.

This alcohol has been suggested for use as a modifier for Geraniol, but it seems that its odor type is not sufficiently different, and its power somewhat deficient.

Prod.: by reduction of *iso*-Citral with Sodium amalgam in alcoholic solution, followed by treatment with Acetic acid.

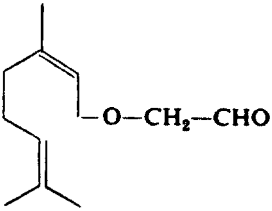
156-106;

## 1428: GERANOXY ACETALDEHYDE

"Geranyl oxyacetaldehyde".
"Peony aldehyde".

Note: The commercial product is not a well defined, single chemical. It contains very large amounts of Citronellyl oxyacetaldehyde, Acetals of both, and other components.

The structure of true Geranoxyacetaldehyde is:



$C_{12}H_{20}O_2 = 196.29$

Colorless viscous oily liquid. Insoluble in water, soluble in alcohol and perfume oils, poorly soluble in Propylene glycol.

Powerful and lasting, sweet-floral, overall green-rosy odor. In spite of comparatively little difference in chemical composition between this aldehyde and the Citronellyl oxyacetaldehyde, there is a distinct difference in odor. The subject material has a deeper, more delicate rosy odor, not as penetrating "aldehydic" as the former.

These odor differences may well be due to the components other than the Geranoxyacetaldehyde itself, since the two oxyaldehydes are present in both products.

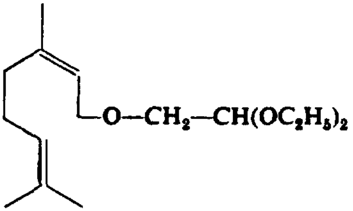
Geranoxy acetaldehyde is used in perfume compositions for variations of the Rose theme, also for "Peony" notes and other delicate nuances, and in Freesia and other sweet floral fragrances.

Prod.: analogous with the preparation of Citronellyl oxyacetaldehyde (see that monograph). One commercial product consists almost entirely of Citronellyl oxyacetaldehyde with minor bouquetting additives and by-products included.

86-54; 156-378;

## 1429: GERANOXYACETALDEHYDE DIETHYLACETAL

*beta*-Hydroxyacetal geranylether.
*beta*-Hydroxyacetaldehyde diethylacetal geranylether.



$C_{16}H_{30}O_3 = 270.42$

Colorless oily liquid. Sp.Gr. 0.90.
B.P. 260° C.

Insoluble in water, soluble in alcohol and oils.

Light and fresh-rosy, green odor with some resemblance to Peony, although greener than the odor of that flower.

This acetal has only little more than academic interest, and the parent aldehyde itself (see previous monograph) is also of doubtful value. It is interesting to notice, however, that these materials were studied more than 35 years ago, yet they have been brought up in the perfumery limelight as late as in the early 1960's. One major disadvantage was probably that a pure Geranoxyacetaldehyde was never produced, and the odor description varied accordingly as new scientists produced the material in various degrees of purity.

The acetal has been suggested for use in perfume compositions, but it is quite sensitive to acid in which it will hydrolyze and Acrolein will be liberated, thus ruining the delicate floral notes.

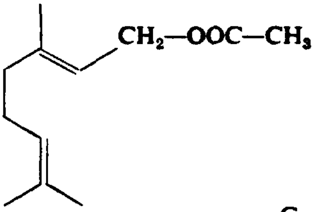
The author believes that this material can be classified as obsolete and of academic interest only.

Prod.: (several methods) e. g.: from Sodium Geraniate and Chloroacetaldehyde diethylacetal (so-called *beta*-Chloroacetal).

31-76; 156-378;

## 1430: GERANYL ACETATE

*2,6*-Dimethyl-*2,6*-octadien-*8*-yl acetate.
Meraneine (A. Boake, Roberts & Co.).



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. B.P. 245° C. Sp.Gr. 0.92.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Glycerin, soluble in Propylene glycol.

Sweet, fruity-floral, rosy, somewhat green and remotely Lavender-like odor of moderate tenacity.

Sweet fruity, overall nondescript taste with notes resembling those of Banana, Pear, Apple and Peach, but not a purely sweet aftertaste.

Widely used in perfume compositions as a sweetener and modifier in floral, fruity, herbaceous and Citrusy fragrance types, usually at a modest level of one to five percent in the concentrated perfume oil, but with great variations according to the purpose of its use. It blends well with Bergamot, Lavender, Rose, Muguet, Wallflower, YlangYlang, Neroli and even Leather, Oriental and other very complex fragrance types.

The ester is used in flavor composition for a great variation of types: Apricot, Apple, Banana, Blackcurrant, Gooseberry, Ginger Ale, Grape, Honey, Lemon, Peach, Pear, Lime, Wine and in various Spice complexes, Berry variations, Floral flavor types, etc., etc.

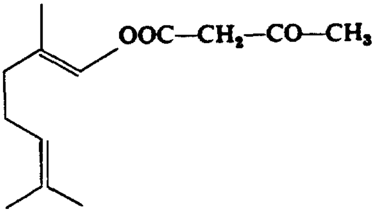
Concentration is normally about 1 to 20 ppm in the finished product. The effect of Geranyl acetate is somewhat stronger than that of Geraniol itself.

G.R.A.S. F.E.M.A. No.2509.

Prod.: by direct esterification of Geraniol with Acetic acid under azeotropic conditions, or with Acetic anhydride under temperature controlled conditions.

4-55; 5-18; 26-558; 31-123; 33-503; 34-806; 77-183; 86-54; 90-258; 106-172; 160-1010; B-II-140; 140-136;

## 1431: GERANYL ACETOACETATE



$C_{14}H_{22}O_3 = 238.33$

Colorless oily liquid. Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet fruity, winey-green "fermented Apple"-like, overall very pleasant odor.

Sweet fruity, ethereal, green-winey taste, reminiscent of Apple or Apple wine.

This ketone is, to the author's knowledge, rarely, if ever, used in perfumery.

It finds some use in flavor compositions, mainly as a trace component in various fruit flavors, not only Apple. It introduces a certain note of natural pleasant "overripe" or "fermented" character to many fruit flavors, and its low rate of volatility makes it a good fixative for the more volatile and common components in these fruit flavors.

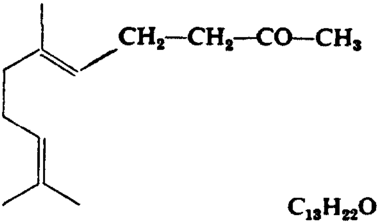
Concentration in the finished product may be in the range of 1 to 10 ppm.

Prod.: (several methods) e. g.: from Geranyl chloride plus Malonic ester. Subsequent careful saponification of the Ethyl ester.

G.R.A.S. F.E.M.A. No.2510.

## 1432: GERANYL ACETONE

*alpha-beta*-Dihydro pseudoionone.
*2,6*-Dimetylundecadien-*2,6*-one-*10*.



$C_{13}H_{22}O = 194.23$

Pale yellowish or almost colorless oily liquid. Color may increase during storage and exposure to air.

Very slightly soluble in water, soluble in alcohol and oils, 10% soluble in Propylene glycol. B.P. 247° C. Sp.Gr. 0.88.

Fresh-floral, light, but rather penetrating, sweet-rosy, slightly green, Magnolia-like odor of moderate tenacity. The odor has some resemblance to that of Rhodinyl formate, yet somewhat sharper. This ketone, which was developed as an intermediate in the synthesis of Nerolidol, has been suggested for use in perfume compositions, particularly in soap perfumes, where its superior stability makes it a very reliable floralizer and sweetener in floral compositions. However, its market cost has not been brought down to a level where it can become really commonplace, large-volume, every-day-used raw material.

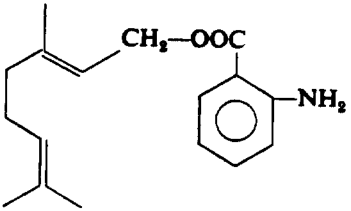
Prod.:

1) from Geraniol via Geranyl chloride and Ethyl geranyl acetoacetate followed by hydrolysis and decarboxylation to Geranyl acetone. (Hoffmann-laRoche prod.).
2) from Linalool with Ethylacetoacetate and Sodium ethylate.

2-1006; 4-55; 5-31; 88-237; 86-55; 156-375; 89-367;

## 1433: GERANYL ANTHRANILATE

Aurantiol (old name, now used for the Schiff's base of Hydroxycitronellal and Methylanthranilate).



$C_{17}H_{23}NO_2$ = 273.38

Yellowish or lemon-yellow, viscous oil.
Sp.Gr. 1.07. B.P. 312° C.

Insoluble in water, soluble in alcohol, miscible with most oils. Almost insoluble in Propylene glycol.

Heavy, sweet, floral and very tenacious odor of Honeysuckle-Frangipanni-type.

The ester is not always a pure chemical, and great variations in odor may be encountered when studying samples from various suppliers.

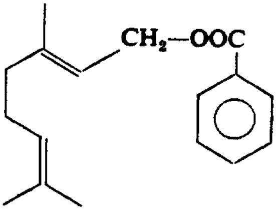
Occasionally used in perfume compositions, mainly in heavy floral types, Honeysuckle, Gardenia, Orangeblossom, occasionally in Jasmin variations, etc.

Prod.:

1) from Isatoic anhydride plus Geraniol.
2) from Methyl anthranilate plus Geraniol with Sodium ethylate.

5-295; 34-1022; 156-43;

## 1434: GERANYL BENZOATE



$C_{17}H_{22}O_2$ = 258.36

Viscous pale straw-colored or almost colorless liquid. B.P. 305° C. Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Faint-rosy, very tenacious, overall mildly floral odor with Ambre-like undertones.

Sweet, generally fruity, overall Apple-like taste in extreme dilution. It is a powerful flavor, pleasant only in concentrations below 2 ppm.

Used in perfume compositions, mostly in floral bases, and particularly in artificial Ylang Ylang. Also in general as a floral fixative which blends well with most floral and many non-floral components, such as Labdanum and artificial Musks, etc.

The ester is also used in a few flavor types, mainly fruity and so-called floral flavors. It is a useful fixative for Mint flavors in chewing gum compositions, etc.

The concentration used is very low, normally about 0.1 to 0.5 ppm in the finished product.

Prod.:

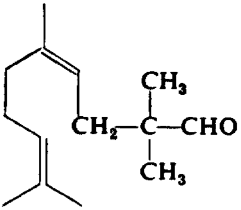
1) from Benzyl chloride and Geraniol with Pyridin catalyst.
2) from Benzoic anhydride and Geraniol with sulfonic acid type catalyst.

G.R.A.S. F.E.M.A. No.2511.

4-55; 86-55; 90-280; 106-174; 36-69;

## 1435: GERANYL-iso-BUTYRALDEHYDE

*2,6,9,9*-Tetramethyl-*2,6*-decadienal.
*2,2,5,9*-Tetramethyl-*4,8*-decadien-*1*-al.



$C_{14}H_{24}O = 208.35$

Colorless or very pale straw-colored liquid.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing and sweet-floral, fruity-rosy odor of good tenacity.

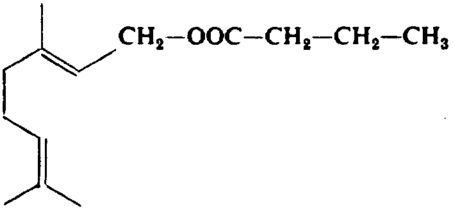
This aldehyde was developed in a research program aiming at new floral type perfume chemicals, and the Lactones, Nitriles and Aldehydes were all included in the search.

A few of the new chemicals have become acknowledged perfume materials, although most of them have never been offered commercially under their proper chemical name.

This aldehyde finds use in perfume compositions as a modifier in Rose and other florals, mainly of the light, green type, including Citrus colognes. The aldehyde suffers from a drawback of poor keeping qualities, and the Nitrile has been developed to overcome this disadvantage (see Geranyl-*iso*-butyronitrile).

## 1436: GERANYL BUTYRATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl-*n*-butyrate.



$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. B.P. 253° C.
Sp.Gr. 0.90.

Insoluble in water, Glycerin and Propylene glycol.

Soluble in alcohol, perfume and flavor oils and in mineral oil.

Sweet, rather heavy, fruity odor reminiscent of Apples, with undertones of red Roses, slightly fatty-oily, but overall very pleasant. Needless to say that traces of free acid are detrimental to this odor picture.

Sweet, deep, fruity taste, remotely reminiscent of Apples, Peaches and wild Strawberries.

This ester is frequently used in perfume compositions, e. g. Cassie, Muguet, red Rose, Geranium, Lavender, Peony, etc. and it is a common ingredient in lipstick perfumes, with or without the conventional Ionones. It blends well with Undecanolide for such purpose, and it shows great power in Citrus fragrances as well as in the above florals. It is comparatively stable towards acid and alkali under normal conditions in functional products.

It finds a great deal of use in flavor compositions for imitation Apple, Cherry, Peach, Pineapple, Orange, Strawberry and various fruit complexes. With Clary Sage oil it often forms base for interesting Pear flavors. The concentration is usually very low, about 1 to 10 ppm in the finished product.

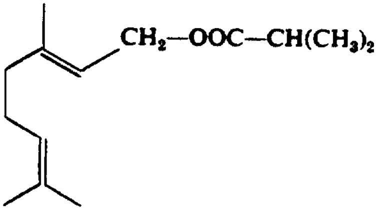
Prod.: from Geraniol and *n*-Butyric anhydride. The water may be removed in azeotropic distillation with the excess Butyric acid formed.

G.R.A.S. F.E.M.A. No.2512.
FCC-1964-827.

4-55; 5-18; 5-233; 26-558; 33-734; 77-186; 90-273; 106-175; 140-140; 156-171; 160-1010; B-II-272;

## 1437: GERANYL-iso-BUTYRATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl-*iso*-butyrate.



$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. Sp.Gr. 0.90.
B.P. 245° C.

Practically insoluble in water, Glycerin and Propylene glycol, soluble in alcohol, mineral oil and most perfume and flavor oils.

Sweeter and more floral than the *n*-Butyrate, less acid (and it has less tendency to become acid), yet overall a fruity odor with rosy character.

Sweet, deep-fruity taste, remotely reminiscent of Strawberry and Peach. Not as Apple-like as the *n*-Butyrate.

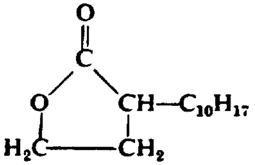
Used in Ambre bases, Chypre, Fougère, Lavender, Geranium, Cassie, Rose, etc. It blends particularly well with materials of balsamic odor type.

The ester finds use in flavor compositions such as Apple (the *n*-Butyrate is preferred here) Peach, Pineapple, Pear, and in various floral and Rose-type flavor complexes.

Prod.: from Geraniol and *iso*-Butyric acid (in excess) by azeotropic type esterification, using the excess acid as a carrier for the water. Other processes utilize a similar azeotropic system, sometimes with Acetic acid as a carrier.

5-233; 31-123; 33-734; 77-186; 90-274;

## 1438: alpha-GERANYL-gamma-BUTYROLACTONE



(See: Geraniol monograph for structure).

$C_{14}H_{22}O_2 = 222.33$

Colorless or pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Almost insoluble in Propylene glycol and Glycerin.

Refreshing, sweet-peachy, but also musky odor of considerable tenacity.

The taste is fruity, Apple-Peach-like, but not purely sweet, and the bitterness is perceptible even through the concentrations near the minimum perceptible of flavor.

This lactone is more of a curiosity than it is an active perfume raw material. It was developed in search of new and interesting odors in the long range of lactones after several successful members had achieved regular use and acceptance by the perfume industry.

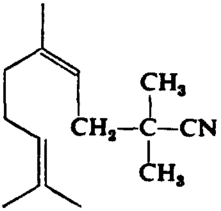
The fragrance effect of the subject material is, in the author's opinion, too weak and uncharacteristic to warrant any further use or experiments with this lactone.

Prod. (several methods) e. g. from Ethylene oxide plus Geranyl malonic ester.

31-170; 159-418;

## 1439: GERANYL-iso-BUTYRONITRILE

Geranyl-*iso*-propylcyanide.
*2,6,9,9*-Tetramethyl-*2,6*-decadienoic acid, Nitrile.
*2,2,5,9*-Tetramethyl-*4,8*-decadiene-*1*-nitrile.



$C_{14}H_{23}N = 205.35$

Colorless or very pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Warm-sweet, floral-herbaceous odor of considerable tenacity.

Less rosy, more pungent than the aldehyde (see Geranyl-*iso*-butyraldehyde), also more powerful and less fruity.

This Nitrile, developed as a stabler version of the aldehyde, should not be considered as a substitute for Geranyl-*iso*-butyraldehyde. The odor difference is too marked, and the two materials may serve entirely different purposes in perfume compositions.

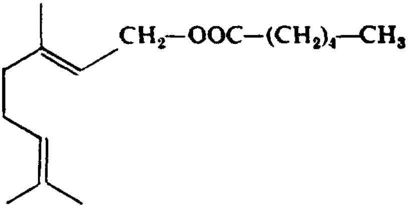
The advantage of the title Nitrile is its stability in air and in mildly alkaline media (soap etc.).

However, it lacks the floral beauty and effect of the aldehyde, and cannot supply such notes. The subject Nitrile is used in heavy floral fragrances, Oriental types, soap and talcum perfumes, etc. but its cost is generally prohibitive for extensive use.

Prod.: from Myrcene, via Myrcene hydrochloride and with *iso*-Butyronitrile, using Sodamide catalyst, to the title material.

## 1440: GERANYL CAPROATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl hexanoate.
Geranyl hexanoate.



$C_{16}H_{28}O_2 = 252.40$

Colorless oily liquid. Sp.Gr. 0.89.
B.P. 290° C.

Insoluble in water, soluble in alcohol and oils.

Fruity Geranium-like with rosy and slightly green undertones. The fruity notes resemble Banana-Pineapple.

Powerful fruity, heavy-sweet taste, pleasant only at concentrations below 5 ppm, and preferably in acid media.

Occasionally used in perfume compositions for variations in the heavier, sweet-exotic floral fragrance types such as Ylang Ylang, Ginger Lily and Wistaria, and also in Magnolia, Peony, Freesia, etc. in more modest amounts.

The ester finds use in flavor compositions for imitation Apple, Pineapple and various Citrus types, as well as "Tutti-frutti" type flavors.

The concentration is usually mere traces, e. g. 1 to 3 ppm in the finished product.

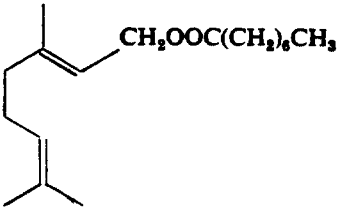
G.R.A.S. F.E.M.A. No.2515.

Prod.: by direct esterification of Geraniol with Caproic acid under azeotropic conditions and with a sulfonic acid type catalyst.

4-56; 34-1230; 36-69; 86-55; 90-279;

## 1441: GERANYL CAPRYLATE

*trans*-*3,7*-Dimethyl-*2,6*-octadienyl octanoate.
Geranyl octylate.
Geranyl octoate.



$C_{18}H_{32}O_2 = 280.45$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

B.P. 304° C. Sp.Gr. 0.88.

Sweet, oily-herbaceous, overall rosy odor with fruity undertones, remotely reminiscent of Apricot and Mango.

Sweet, somewhat oily-fruity taste of considerable power. Pleasant only at concentrations below 5 ppm, rather 2 or 1 ppm.

The author is not aware of this chemical being used in perfumes. It could find some use as a modifier in heavy florals as well as in the more delicate types such as Peony and Freesia or Appleblossom (not the conventional brutal offspring of a Hyacinth!!), etc.

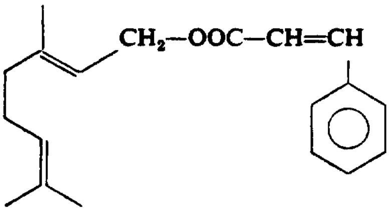
The ester could find some use in flavor compositions, e. g. in the tropical fruit imitations: Mango, Passionfruit, Pineapple, etc.

Prod.: by direct esterification of Geraniol with Octanoic acid under azeotropic conditions, and using a sulfonic acid type catalyst.

90-281;

## 1442: GERANYL CINNAMATE

*trans*-*3,7*-Dimethyl-*2,6*-octadien-*8*-yl-*beta*-phenylacrylate.
Geranyl-*3*-phenylpropenoate.



$C_{19}H_{24}O_2 = 284.40$

Viscous, pale straw-colored or almost colorless liquid.

Sp.Gr. 1.08. B.P. 384° C. (decomposes).

Insoluble in water, soluble in alcohol, miscible with most oils.

Mild and sweet Ambre-Rose type odor with soft, balsamic undertones. There is a noticeable difference between samples from one or the other supplier, particularly if different methods of production have been applied.

Balsamic-rosy, but not quite sweet taste. Pleasant at about 1 ppm but is too weak at that concentration for practical effects.

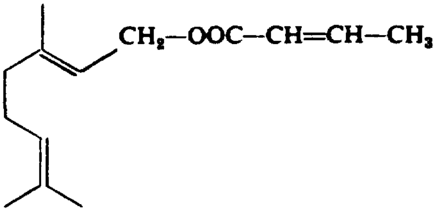
This rare ester finds occasionally use in mild floral fragrances or heavy and sweet Oriental or balsamic type bases. It has some of the Ambre notes of a good grade Asiatic Styrax, and it blends very well with Labdanum derivatives to emphasize such notes. It is also an interesting modifier for Oakmoss in cases where a Coumarinic companion note is undesirable, or a spicy moss not wanted. It maintains the lasting effect of the Oakmoss but keeps it continously soft and sweet instead of dry or woody.

Prod.: from Cinnamyl chloride plus Geraniol with a catalyst.

34-462; 36-82; 90-283;

## 1443: GERANYL CROTONATE

Geranyl-*2*-butenoate.
Geranyl-*alpha*-crotonate.



$C_{14}H_{22}O_2 = 222.33$

Colorless or pale straw-colored liquid.

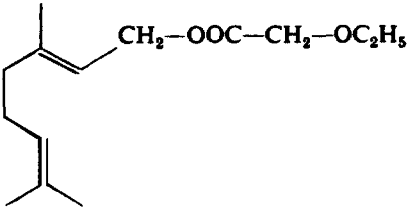
Insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, sweet odor with a rosy-woody undertone and good tanacity.

This ester, although only rarely offered commercially, should have good possibilities in artificial Geranium and in general in perfumes of herbaceous-floral, sweet character. Yet, the ester blends excellently with woody odors, with Clary Sage and Lavender, etc. It is furthermore an excellent extender for Zdravetz oil in the rare cases where this oil is used and its notes should be modified.

Prod.: by direct esterification of Geraniol with *2*-Butenoic acid using azeotropic conditions.

## 1444: GERANYL ETHOXYACETATE



$C_{14}H_{24}O_3 = 240.35$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

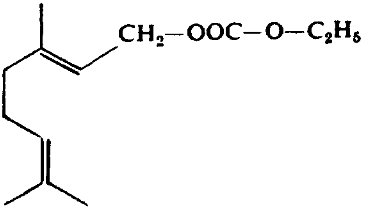
Rosy and somewhat green odor, milder than Geranyl acetate and much less fruity.

The author is of the opinion that this ester has little, if any application in perfumery or interest to the creative perfumer. It has some academic interest for the subject of studying the relationship between odor and chemical structure, influence of certain radicals upon the odor type, etc.

Prod.: by direct esterification.

31-159;

## 1445: GERANYL ETHYL CARBONATE



$C_{13}H_{22}O_3 = 226.32$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and mellow, rosy, and warm, tenacious odor.

Sweeter than Geraniol, but not fruity like Geranylacetate, rather mellow in an almost musky way.

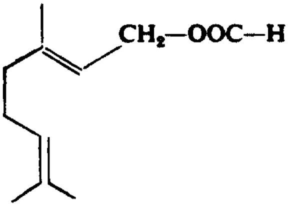
This ester, although just a member of a long line of Ethylcarbonates, many of which are listed in this work, is rarely offered commercially under its proper chemical name. In fact, the author has not yet seen any of these "Ethylcarbonates" listed in a price list from a manufacturer of perfume chemicals.

Some of these materials have become quite popular (within the company where they may be manufactured), since they offer a generally smoother and mellower version of the parent alcohol, as if accompanied by a discrete winey-musky note.

Prod.: from Geraniol and Ethylalcohol with Phosgene (Carbonyl chloride).

## 1446: GERANYL FORMATE

*trans*-*3*,*7*-Dimethyl-*2*,*6*-octadienyl formate.



$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. Sp.Gr. 0.92. B.P. 216° C.

Insoluble in water, Propylene glycol and Glycerin. Soluble in alcohol and oils, also in mineral oil.

Fresh, but somewhat dry, green-rosy, "leafy" odor, diffusive and remotely fruity. Reminiscent of Rose, Geranium, Bergamot, Neroli, and with an intriguing note of Apple-skins and Ginger.

Sweet green-fruity, slightly woody-spicy taste at low concentration. The ester is frequently used in perfumes, mainly in the lighter portions or in the topnote compositions for Rose, Tuberose, Neroli, Citrus colognes, Lavender, etc.

It is also used in flavor compositions for imitation Apple, Apricot, Blackcurrant, Gooseberry, Peach and in various fruit complexes and Citrus compositions. It is quite powerful and the normal concentration in the finished product is about 1 to 10 ppm.

Prod.: by formylation of Geraniol, e. g. by using Formic acid and Geraniol in cold reaction, or by adding Acetic anhydride to the mixture.

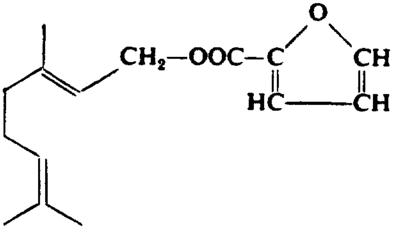
G.R.A.S. F.E.M.A. No.2514.

FCC 1964-829.

4-56; 5-17; 26-558; 77-179; 86-55; 90-242; 106-176; 160-1010; B-II-23; 140-132;

## 1447: GERANYL FUROATE

Geranyl pyromucate



$C_{15}H_{20}O_3 = 248.33$

Colorless or pale straw-colored liquid. Almost insoluble in water, soluble in alcohol and oils.

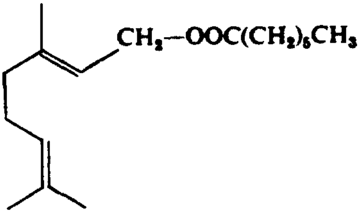
Sweet-herbaceous, woody, slightly fruity (fruit-preserve-like) odor of good tenacity. This ester has notes resembling Geranium, but it is much softer and lacks the green freshness of Geranium materials.

Geranyl furoate has been suggested for use in perfume compositions. However, it is rarely offered commercially and the ester does not seem to have any unusual odor characteristics or effects tempting enough to make it a commonly desired chemical.

Prod.: by direct esterification of Geraniol with Furoic acid using azeotropic conditions.

## 1448: GERANYL HEPTOATE

Geranyl heptylate.



$C_{17}H_{30}O_2 = 266.43$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Mild and fresh-floral-fruity odor of good tenacity. More fruity than floral, the fruity notes resembling Peach and Apricot.

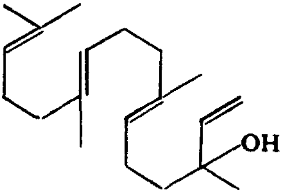
Fruity Apricot-like taste, but not quite sweet.

Has been suggested for use in perfume compositions, but this ester seems to be too rare in the trade to find a wider use, and its odor characteristics are not sufficiently unusual to warrant a preference for this ester.

Prod.: by direct esterification of Geraniol with Heptanoic acid under azeotropic conditions.

## 1449: GERANYL LINALOOL

A naturally occurring unsaturated C-20 alcohol.
*3,7,11,15*-Tetramethyl-*1,6,10,14*-hexadecatetraen-*3*-ol.



$C_{20}H_{34}O = 290.49$

Viscous colorless liquid. Sp.Gr. 0.89.
B.P. over 340° C.

Insoluble in water, soluble in alcohol, miscible with most perfume oils.

Mild and sweet, delicately green-floral odor with a slightly woody undertone, yet not an overall dry odor.

Its tenacity is probably its greatest asset, and its odor performance resembles that of Farnesol to a certain degree in that the odor at first seems extremely weak, then it increases in volume – rather than in strength – until it shows a rich, still delicate fragrance of outstanding tenacity.

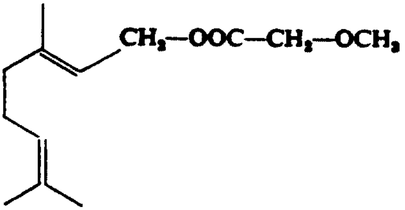
This alcohol, only recently available on a commercial scale at an attractive price, is used in artificial flower absolutes and in the more delicate and long-lasting floral perfume types, such as Muguet or Jonquil, also in Tuberose. It blends excellently with the conventional floralizers in these fragrance types, and its delicate odor is usually brought up to a more perceptible level when this alcohol is incorporated in a light, floral base.

It is, in the author's opinion, one of the most valuable contributions to the perfumers "library" in the past decade.

Prod.: in the process of making synthetic Vitamin E via Farnesol. See also *iso*-Phytol, which can be described as a Hexahydro geranyl linalool.

88-363;
Hoffmann-laRoche sample;

## 1450: GERANYL METHOXY ACETATE



$C_{13}H_{22}O_3 = 226.32$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Very faint and mild rosy odor with such a lack of floralness that the odor is often described as "musky" (a term often used for weak odors or nondescript, sweet odors).

Prod.: by direct esterification of Geraniol with Methoxy acetic acid.

31-159;

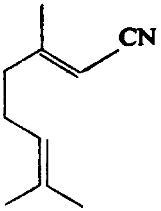
## 1451: GERANYL NITRILE

The commercial name is somewhat misleading since the material is the Nitrile of Geranic acid.

Gerano nitrile.

Citralva.

*3,7*-Dimethyl-*2,6*-octadiene-*1*-nitrile (*cis*- and *trans*-isomers).



$C_{10}H_{15}N = 149.24$

Almost colorless or very pale yellowish oily liquid. B.P. 222° C. Sp.Gr. 0.87.

Practically insoluble in water, soluble in alcohol and oils.

Penetrating and powerful, oily-green, lemony-fresh odor with some resemblance to that of Citral, but overall harsher, not as sweet and not as natural in its notes.

Powerful lemony, but also somewhat "metallic" and not expressly sweet taste – in dilutions below 5 ppm. It should be noted that this material has a poorer effect in acidified aqueous medium than the effect obtained with Citral under similar conditions.

This material – a member of a large family of Nitriles developed for perfumes since Georges Igolen in the late 1940's produced Nitriles parallel to alifatic aldehydes, – has been praised for its Citral-like effect and comparative stability under mildly alkaline conditions (e.g. soap).

It is however, not possible to substitute Citral in an already established formula with this Nitrile. The odor can be approached with a somewhat lower ratio of the Nitrile, but the natural Lemon-sweetness must be obtained from other chemicals.

Due to its chemical Nature, this material is not stable in flavors where acid is incorporated.

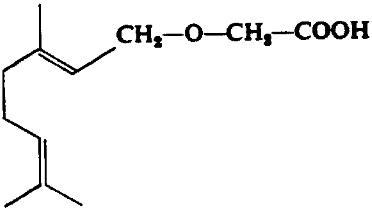
Prod.:

1) from Geranialoxime with Acetic anhydride.
2) from Geranyl chloride and Sodium cyanide.

6-144;
(See also: *3,7*-Dimethyloctanal-*1*).

## 1452: GERANYL OXYACETIC ACID

Geranoxyacetic acid.



$C_{12}H_{20}O_3$ = 212.92

Pale yellowish liquid. Very slightly soluble in water, soluble in alcohol and oils.

Faintly rosy, but overall fatty-acetic odor, remotely reminiscent of Acetic acid.

Sharp and pungent taste.

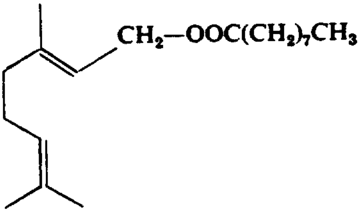
Apart from some possible application in the reconstruction of certain essential oils, this acid has probably very little use in perfumery.

Prod.: from Glycollic acid and Geraniol.

31-158;

## 1453: GERANYL PELARGONATE

Geranyl nonanoate.
Geranyl nonylate.
*trans-3,7*-Dimethyl-*2,6*-octadienyl nonanoate.



$C_{19}H_{34}O_2$ = 294.48

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

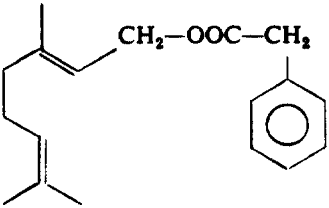
Fresh and leafy, Rose- and Geranium type odor, overall more resembling Geranium. Mild, oily winey undertones.

This ester, not often found in the commercial price lists, could find some use in perfume compositions as a modifier for lower alifatic Geraniol esters, not only in Geranium compositions, but in perfumes where the fruity-winey middle notes of Geranium, other than those deriving from the "Rhodinol" section, may be desired.

Prod.: by direct esterification of Geraniol with Nonanoic acid under azeotropic conditions.

## 1454: GERANYL PHENYLACETATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl phenylacetate.



$C_{18}H_{24}O_2$ = 272.39

Colorless or pale straw-colored, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Soft and very sweet, tenacious, mildly floral-honeylike almost herbaceous odor with Geranium-like undertones and variable amounts of animal notes. Trace impurities, particularly the two components from which the ester is prepared, may strongly influence this odor picture. Geraniol and Phenylacetic acid are both stronger odorants than this ester, and the acid in particular will introduce overpowering animal-honey-like notes, while poor distillation conditions, too high temperature, etc., may also increase the "animal" notes.

Powerful, sweet, mainly honey-like taste with a heavy-fruity note.

This ester is used in perfume compositions of the type where floral notes and Honey-notes are compatible, e. g. Hyacinth, Lily, Narcissus, Lilac, Jonquil, etc. and in variations of Oriental fragrance types.

The ester finds some use in flavor compositions such as imitation Apricot, Peach, Honey, and in various fruit complexes.

The concentration used is normally as low as 1 to 10 ppm in the finished product.

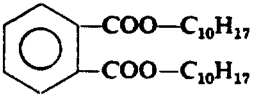
Prod.: from Geraniol and Phenylacetyl chloride. The latter is usually prepared from Phenylacetic acid and Thionyl chloride.

G.R.A.S. F.E.M.A. No.2516.

4-56; 5-270; 36-82; 34-246; 86-55; 106-177;

## 1455: GERANYL PHTHALATE

Di-geranyl phthalate.



$C_{28}H_{38}O_4 = 438.61$

Colorless viscous oil. Insoluble in water, soluble in alcohol and oils.

Practically odorless when pure.

The author is of the opinion that this material, probably developed in an attempt to make a fixative with a mild, universally applicable odor, is of very little value as a perfume material.

Phthalates, other than Diethylphthalate, have more or less been abandoned and are no longer desirable as perfume materials, not even as solvents.

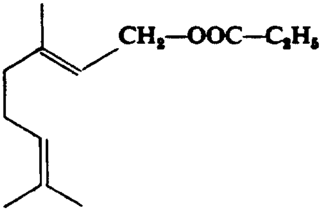
Subject material has been mentioned in the perfumery literature as a perfume material.

Prod.: from Phthalic anhydride and Geraniol with a catalyst.

4-56;

## 1456: GERANYL PROPIONATE

*trans*-3,7-Dimethyl-2,6-octadienyl propionate.



$C_{13}H_{22}O_2 = 210.32$

Colorless liquid. Sp.Gr. 0.90. B.P. 253° C.

Almost insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol, mineral oil and perfume oils, almost insoluble in Glycerin.

Sweet, fruity-rosy, warm and almost balsamic-Grape-like odor with a leafy-floral undertone and moderate tenacity.

Sweet, rather heavy, fruity-floral taste with a slightly bitter aftertaste.

This ester is used in perfume compositions mainly to introduce fruity notes in or near the topnote composition. It may also find some use in heavy florals with pronounced fruity tones, such as Gardenia, Passionflower, etc. but even in Geranium, Lavender and naturally in variations of Rose bases it finds extensive application.

Geranyl propionate is a powerful additive in many types of flavors, particularly in Apple, Apricot and Pear, also in Pineapple, Honey, Berry complexes and fruity types.

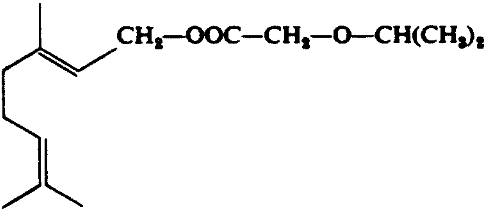
The concentration used is equivalent to about 1 to 5 ppm in the finished product, except in chewing gum where it may go as high as 70 ppm.

Prod.: by direct esterification of Geraniol with Propionic acid under azeotropic conditions, or with Propionic anhydride.

F.E.M.A. No.2517. F.C.C.-1964-831.
G.R.A.S.

4-56; 33-622; 86-55; 90-270; 106-178;

## 1457: GERANYL-iso-PROPOXYACETATE



$C_{15}H_{26}O_3 = 254.37$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Very weak, green and rosy odor.

Very weak, nondescript taste.

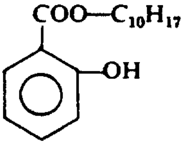
Although this material has been recommended for its fragrance, the author is of the impression that it has lost its importance – if it ever had any – as a fragrance material. It is simply too mild and nondescript, and the mild odor is not due to a particularly high boiling point.

Prod.: by direct esterification.

31-159;

## 1458: GERANYL SALICYLATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl-*ortho*-hydroxybenzoate.



$C_{17}H_{22}O_3 = 274.36$

Colorless viscous liquid. Insoluble in water, soluble in alcohol and oils.

Virtually odorless when pure, but the ester does contribute sweet, rosy-balsamic notes to a composition when lower boiling materials are present.

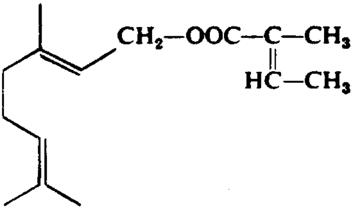
It finds a little use as a fixative, or a "so-called fixative" in the common definition of at least four types of fixatives.

Prod.: from Geranyl chloride plus Sodium salicylate.

4-56; 34-788; 86-55;

## 1459: GERANYL TIGLATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl-*trans-alpha-beta*-acrylate.



$C_{15}H_{24}O_2 = 236.36$

Colorless oily liquid, practically insoluble in water. Soluble in alcohol and oils.
B.P. 269° C.

Very pleasant, sweet-herbaceous, Geranium-like and fruity odor. The Geranium notes resemble the middle and late notes in natural Geranium, and the fruity notes are deep, almost "jam-like", tenaciously sweet, yet an overall refreshing odor with a touch of leafyness. The author finds that the commercial marketing of this material is one of the more encouraging and welcome happenings to the perfume industry during the past decade.

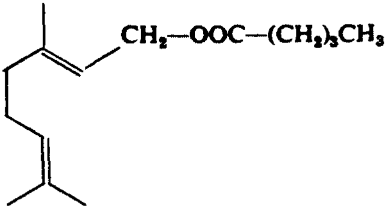
The ester finds increasing use in perfumery (as its price becomes more attractive) not only in artificial Geranium, but widely in cosmetic Rose fragrances, in Lavender bouquets, Oriental bases, etc.

Prod.: from Geraniol and Tiglyl chloride in an inert volatile solvent and using a Pyridine type catalyst.

7-189; 7-192; 86-55; 90-278;
(Sample: Fritzsche Bros. Co., Inc.).

## 1460: GERANYL VALERATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl pentanoate.



$C_{15}H_{26}O_2 = 238.37$

Colorless liquid. Sp.Gr. 0.89. B.P. 291° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, fruity, almost Pineapple-like and Apple-peel-like odor with rosy-tobaccolike, herbaceous undertones.

Traces of free acid will seriously change the odor picture of this ester.

Fruity, Apple-like, somewhat herbaceous and not very sweet taste.

This ester finds some use in perfumery for Lavender, Geranium, Appleblossom, Sweet Pea, Freesia and Peony, and in various Rose types.

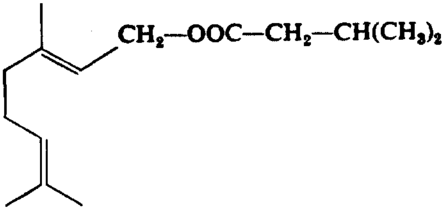
It is also used now and then in flavors, mainly Apple and Peach imitations, and in tobacco flavoring.

Prod.: by direct esterification of Geraniol with *n*-Valeric acid using azeotropic conditions.

4-56; 33-933; 86-55; 90-276;

## 1461: GERANYL-iso-VALERATE

*trans-3,7*-Dimethyl-*2,6*-octadienyl-*iso*-pentanoate.



$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Fruity, Apple-like, somewhat rosy odor with distinctly herbaceous-sweet undertones, also reminiscent of "overripe fruit".

Powerful, fruity-rosy, but not quite sweet taste. Herbaceous aftertaste.

The *iso*-valerate seems to be slightly more popular than the *n*-ester. It finds use in perfumes as a modifier for lower alifatic esters of Geraniol, and in Oriental fragrance types where it blends excellently with Opopanax, Patchouli and Phenylacetates, etc.

Its tenacity is quite good, and its overall odor performance is a pleasant one, provided the ester is absolutely acid-free.

In flavors, the ester finds use as a modifier for Apple imitations, Pineapple, Lime, Peach, and in a number of Berry formulations. It is also used in tobacco flavorings.

Normal concentration is about 4 to 10 ppm in the finished product.

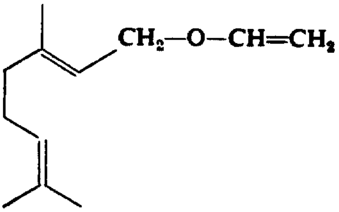
Prod.: by direct esterification of Geraniol with *iso*-Valeric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2518.

156-171; 33-934; 4-56; 86-55;

## 1462: GERANYL VINYL ETHER

Vinyl geranyl ether.



$C_{12}H_{20}O = 180.29$

Colorless oily liquid. Insoluble in water, soluble in alcohol, miscible with perfume oils.

Fresh, "leafy"-green odor with some resemblance to the lighter "Rose" acetals. Warm-rosy undertones.

This ether has been suggested for use in perfume compositions, and particularly in soap perfumes, where the stability of the ether, and its insolubility in water should give it some advantages over Geraniol and its nearest derivatives.

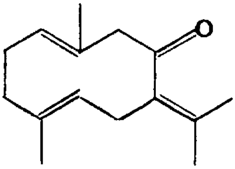
The ether is not very commonly offered commercially, but it is occasionally available from manufacturers who have facilities for undertaking the Acetylene-Vinylether reaction.

Prod.: from Geraniol and Acetylene under pressure with a catalyst, usually an oxide or hydroxide or alkoxide of Sodium, Potassium, Silver, etc.

## 1463: GERMACRONE

*1,7*-Dimethyl-*4-iso*-propylidene cyclodecadien *-6,10*-one.

This material was formerly known under the name: Germacrol.



$C_{15}H_{22}O = 218.34$

White crystals, melting at 56° C. Sp.Gr. 0.97 (liquid).

Very faint, sweet-woody, somewhat herbaceous odor of extraordinary tenacity.

This material which is very rarely offered as such, occurs in very high amounts in one rare essential oil. It could find use as a modifying fixative in Ambre, Chypre and mossy fragrance types or bases, but it has been possible in most cases to use the essential oil itself for such effects.

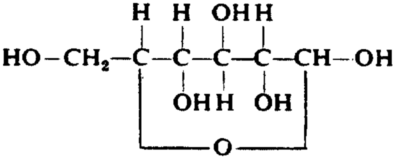
It blends very well with the Ionones, Geranium, Methylnonyl-acetaldehyde, Ambergris tincture, Vetiver- and Cedarwood derivatives, etc.

Prod.: by isolation (freezing) from Bulgarian Zdravetz oil. This oil contains about 50 to 60% of the ketone.

89-419; 104-672;

## 1464: GLUCOSE

Dextrose (name for the pure chemical).
Hexose.
Cerelose.
Grape sugar.
Corn sugar.
Dextropur (one of many brand names for pure material).
*dextro*-Glucose (commercial, impure Dextrose))
– and many other names.



$$\mathrm{HO{-}CH_2{-}\overset{H}{\underset{|}{C}}{-}\overset{H}{\underset{OH}{C}}{-}\overset{OH}{\underset{H}{C}}{-}\overset{H}{\underset{OH}{C}}{-}\underset{|}{CH}{-}OH}$$

$$\mathrm{\llcorner\_\_\_\_ O \_\_\_\_\lrcorner}$$

$C_6H_{12}O_6 = 180.17$ (anhydrous)

White crystalline or granular material, melting at 146° C.

Most commercial brands contain 1 Mol. $H_2O$: $C_6H_{12}O_6, H_2O = 198.18$.

This material melts at 86° C.

45% soluble in water at room temperature. 2% soluble in alcohol, practically insoluble in oils.

Virtually odorless. Sweet taste with a peculiar, initially cool mouthfeel, followed by a warmer feeling. Technical or poor grades have a slightly caramellic odor and taste.

The sweetening effect is about 0.75 times that of cane sugar.

A food additive rather than a flavor material, Glucose lends one of the basic tastes – sweet – to the majority of all candy products, many sherbet ices, soft and alcoholic beverages, cordials, etc. It is marketed as a crystalline powder, hydrous or anhydrous, or as a supersaturated syrup, a very viscous, barely pourable, colorless material. Being resistant to mild acid, it is preferred over cane sugar in all candy and sherbets where acid is a necessary ingredient for the flavor (Citrus, Pineapple, etc.). Its sweetness and its viscosity remain unchanged under such conditions.

Prod.: by Hydrochloric acid hydrolysis of Corn starch under pressure (about 2 atmospheres) and heat (about 22 minutes).

G.R.A.S. F.E.M.A.

26-572; 66-1252; 100-484; 124-58; 160-1012; B-I-879;

## 1465: GLUCOSE PENTA-ACETATE

1) Penta-acetyl-*alpha-dextro*-glucose.
2) *beta*-Penta-acetyl-*dextro*-glucose.

1) $C_6H_7O(OOC—CH_3)_5$ M.P. 113° C.
   0.15% soluble in water.
2) $C_6H_7O_6(OC—CH_3)_5$ M.P. 131° C.
   0.09% soluble in water.

About 1.2% soluble in alcohol.

Almost insoluble in oils.

$C_{16}H_{22}O_{11} = 390.35$

Needlelike crystals, white or colorless.

Virtually odorless, pronounced bitter taste.

Glucose-penta-acetate is used as a bitter principle in food products, mainly spice blends, condiments, alcoholic beverages, etc. The concentration used is equivalent to about 100 to 1500 ppm in the finished consumer product.

According to Moncrieff (literature 30, 31 and 159) it is apparently common that sweet taste decreases, while bitter taste increases as Hydroxyl-groups are substituted with Acetyl groups in the molecule.

The penta-acetate has a bitterness which is still comparatively pleasant, while the Octa-acetate – used for denaturing of alcohol – is unpleasantly astringent-bitter in its effect.

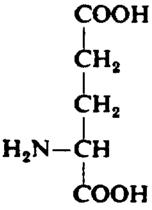
Prod.: from *dextro*-Glucose by Acetylation.

G.R.A.S. F.E.M.A. No.2524.

26-560; 66-1254; 160-1012; BXXX-I-119;

## 1466: Laevo-GLUTAMIC ACID

*L-dextro*-Glutaminic acid.
*dextro-alpha*-Aminoglutaric acid.
*2*-Aminopentane dioic acid.
*1*-Aminopropane-*1,3*-dicarboxylic acid.
Glutaminol.
Glutaton.
– and many other trade names.



$$HOOC—CH_2—CH_2—CH(NH_2)—COOH$$

$C_5H_9NO_4 = 147.14$

White or colorless plate-like crystals.
M.P. 212° C. (decomposes).

0.9% soluble in water, almost insoluble in alcohol and oils. About 5% soluble in hot water.

This monograph describes the naturally occurring *dextro*-rotatory form which has a *Laevo*-configuration. The synthetic (racemic) product is known, and so is the *laevo*-rotatory form with a *Dextro*-configuration.

The acid itself is not much used in foods, but its esters, salts and the hydrochloride are all known and used as food additives. The Sodium salt is described in this work under Monosodium glutamate, the ethyl ester under Diethyl glutamate. The hydrochloride, which is used in Medicine as an acidifier for the human digestive system, has found some use as a flavor enhancer in beverages.

Only the natural form, the *dextro*-rotatory *Laevo*-Glutamic acid, has flavor enhancing effect, and it is used mainly as a Monosodium salt.

The acid itself has a very faint odor resembling that of yeast or freshly baked bread (but much weaker), and its taste in aqueous media is mild, meat-like, rather sweet. The effect of the Sodium salt is greatly improved in presence of Sodium chloride (salt).

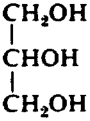
Prod.:
1) from Wheat gluten by treatment with hot Hydrochloric acid (concentrated). The hydrochloride is reacted with Aniline to form the *d*-Glutamic acid, avoiding racemization.
2) synthetic – from Laevulic acid (academic interest only).

G.R.A.S. (when used as a salt substitute).

66-1115; 160-1012; B-IV-488; 26-560;

## 1467: GLYCERIN

Glycerol.
*1,2,3*-Propane triol.
Trihydroxypropane.



$$\begin{array}{l} CH_2OH \\ | \\ CHOH \\ | \\ CH_2OH \end{array}$$

$C_3H_8O_3 = 92.10$

Commercial grades usually contain at least 5% water.

Colorless viscous liquid. Sp.Gr. 1.25 (1.26 when anhydrous).

B.P. 290° C. (decomposes). Miscible with water, Propylene glycol and alcohol in all proportions. Almost insoluble in oils or hydrocarbons. May solidify in the cold, but only at very low temperature and long exposure. Melts again at 18° C.

Commercial grades usually have a faint odor, which can be due to absorbed impurities from the outside, from the container, etc. It can also derive from catalysts, pyrogenated impurities, etc. from distillation or bleaching processes. Amine-like odors, often described as "mouse-urine-like" are not uncommon in Glycerin made in the soap processing, while the "synthetic" Glycerin may have odors, sometimes described as resembling that of "wet cardboard or paper".

The taste is sweet, and the mouthfeel is warm (at high concentration). The sweetening effect is about 0.6 times that of cane sugar.

Glycerin is a useful co-solvent for Vanillin and other Vanilla flavor ingredients, and it is used in flavors for baked goods because of its stability towards heat. In alcoholic beverages it may be used to increase the "body" of the Liqueur or cordial. It behaves like a Carbohydrate in the human body, and the human tolerance is in excess of 100 grams of Glycerin per day.

It is also used as a plasticizer in various types of Gelatin-candy or Licorice candy, etc. and in Fondant fillings.

The concentration is on an average about 500 to 1300 ppm in the finished consumer product. More specifically, it may be up to 6000 ppm in chewing gum, up to 23000 ppm in toppings and as high as 400.000 ppm in extracts.

G.R.A.S. F.E.M.A. No.2525.

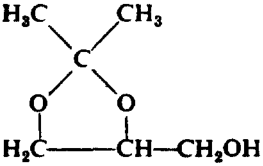
Prod.:

1) by hydrolysis of facts in the manufacture of soaps, etc.
2) as a by-product in the sugar fermentation in presence of Sodium Sulfite (a rather rare method).
3) synthetically from Propylene (from oil gas) via Allyl chloride and its Chlorohydrin to Glycerin by alkaline hydrolysis.

26-560; 66-1013; 77-174; 100-489; 160-1014; B-I-502; 140-128;

## 1468: GLYCEROL DIMETHYLKETAL

"Solketal".
Acetone glycerol.
*1,2-iso*-Propylidene glycerol.
*2,2*-Dimethyl-*4*-hydroxymethyl-*1,3*-dioxolane.
*2,2*-Dimethyl-*1,3*-dioxolane-*4*-methanol.
This monograph describes the *1,2*-ketal, not the *1,3*-ketal, or the mixture.



$C_6H_{12}O_3 = 132.16$

Viscous colorless liquid. B.P. 194° C. Sp.Gr. 1.06.

Miscible with water, alcohol, oils, including terpenes, etc.

When absolutely pure, it is almost odorless. Certain commercial grades have a musty-sweet, slightly earthy odor, somewhat similar to that observed in Hexylene glycol. Its taste is slightly bitter if the concentration is higher than 100 ppm.

Although the subject material can not be classified as a flavor or perfume ingredient, it is mentioned in this work because it is an unusually good solvent for many perfume and flavor materials, and it is in most countries accepted as harmless in food flavors. There are even statements to the effect that it is less irritating than Ethylalcohol.

In view of the extreme scarcity of odorless and tasteless solvents of low toxicity, the title material should have very good possibilities.

Prod.: from Glycerol and Acetone by various means of treatment:

1) in presence of Toluolsulfonic acid.
2) in presence of Sulfamic acid.
3) in presence of dry Hydrogen chloride.
4) in presence of Cupric sulfate at low temperature.

In all cases in absence of water, i. e. using anhydrous Glycerol.

66-1031; 100-967;

## 1469: GLYCERYL MONO-OLEATE

Mono olein.
Glyceryl-*1*-mono oleate.

$C_{17}H_{33}—COO—CH_2—CHOH—CH_2OH$

$C_{21}H_{40}O_4 = 356.55$

Pale yellowish oily, somewhat viscous liquid, solidifying in the cold, melting again below room temperature.

Glyceryl mono-oleate exists in several modifications with different melting points and physical characteristics.

High-grade products have only a faint, sweet-oily odor and a mild, fatty-oily taste. The presence of considerable amounts of free Oleic acid presents a hazard when the acid eventually decomposes slightly (turns "rancid") and produces unpleasant by-odors.

Mono-olein is used as a food additive, mainly in baked products as part of the shortening. During the baking, most of the Mono-oleate is transformed into Di- or Tri-oleate, a process which will take place at temperatures higher than 140° C.

The concentration used is equivalent to about 600 to 2000 ppm in shortening and baked goods.

Prod.: by esterification of Glycerin with Oleic acid in presence of a suitable catalyst.

G.R.A.S. F.E.M.A. No.2526.

66-1016; 160-1016;

## 1470: GLYCERYL MONOSTEARATE

Glyceryl-*l*-monostearate.
Glyceryl mono-octadecanoate.
*alpha*-Monostearin.
The commercial product contains significant amounts of Glyceryl monopalmitate.

$C_{17}H_{35}—COO—CH_2—CHOH—CH_2OH$

$C_{21}H_{42}O_4 = 358.57$

Solid white mass or flaky white crystals of waxy texture. M.P. 58° C. (other modification melts at 82° C.).

Insoluble in water, soluble in hot alcohol and oils.

Emulsifiable with water in the presence of surfactants (e. g. soap).

Glyceryl monostearate is used for the same purposes as Glyceryl mono-olein, and it has some advantages in having less odor and no tendency to turn rancid. It will also form Di- and Tri-stearates when heated beyond 140° C.

The concentration used in baked goods or in shortening is equivalent to about 100 to 2000 ppm in the finished product.

Prod.: by partial esterification of Glycerin with Stearic acid.

G.R.A.S. F.E.M.A. No.2527.

26-562; 100-490; 160-1016; B-II-380;

## 1471: GLYCYRRHIZIN, AMMONIATED

Ammonium glycyrrhizate.
Ammonium salt of Glycyrrhetinic acid glucoside.

$C_{42}H_{61}O_{16}—NH_4 = 839.99$

Light brown or pale amber-colored shiny crystals or flakes.

Soluble in aqueous alkali or in a weak Ammonia solution. Almost insoluble in cold alcohol, soluble in hot alcohol. Insoluble in oils.

Very faint, sweet caramellic-rootlike odor.

Intensely sweet taste. In higher concentrations producing a slightly burning sensation in the back of the mouth and in the throat, shortly after the sweet taste. In extreme dilution there is only a sweet taste.

Glycyrrhizin (ammoniated) as such is not widely used in flavors, but the impure Glycyrrhizin, the Licorice extract, is very widely used in making candy. For special purposes, the Glycyrrhizin itself may be used as a sweetener. It has several drawbacks, however: the sweet taste is inactivated in the presence of acid. And the material introduces a strong color (amber or brown) to the products in which it is used. If it were not for these drawbacks, Glycyrrhizin could find use as a sweetener in non-nutritive beverages, etc.

The normal concentration used is about 5 to 60 ppm in the finished consumer product.

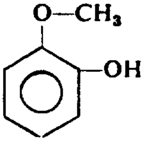
Prod.: Glycyrrhizic acid is extracted from the rhizomes of Glycyrrhiza glabra (mainly from the Spanish variety: typica) in a 6 to 14% yield. The Ammonium salt is the subject article.

G.R.A.S. F.E.M.A. No.2528.

100-492; 124-160; see also: 104-366;

## 1472: GUAICOL

*ortho*-Methoxyphenol.
*ortho*-Hydroxy anisole.
(Pyro)catechol monomethylether.
*l*-Oxy-*2*-methoxybenzene.
Methylcatechol.



$C_7H_8O_2 = 124.14$

Colorless prismatic crystals. Darkens in air and daylight. M.P. 28° C. – melts to a colorless oily liquid. B.P. 205° C. Sp.Gr. 1.13.
1.7% soluble in water, 50% soluble in Glycerin, soluble in Propylene glycol, miscible with alcohol and oils.

Powerful smoke-like, somewhat medicinal odor, sweeter than the prototype phenolic odor.

Warm, medicinal and somewhat sweet taste, but accompanied by a burning sensation, even in high dilution.

This Phenolether is used in perfume compositions in very modest amounts for certain floral types, such as Cananga and YlangYlang, minute traces in Lilac, Narcissus, Lily, etc. It is also useful in Carnation, while somewhat higher proportions can be used in Spice complexes. It is accompanied by the usual drawbacks of simple Phenols – sensitivity to alkali, air, daylight, iron, etc.

Guaiacol finds some application in flavor compositions, such as imitation Coffee, Vanilla, Whisky (smokey effect), Tobacco, Rum, etc. and in many fruit and Spice complexes.

The concentration used is normally very low, about 1 ppm in the finished product.

The toxicity of Guaiacol is estimated to be somewhat lower than that of Phenol.

G.R.A.S. F.E.M.A. No.2532.

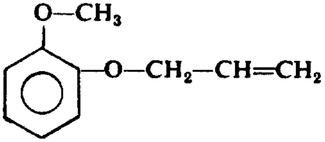
Prod.:
1) from *ortho*-Nitrophenol via *ortho*-Anisidine and the Diazo-compound.
2) from Pyrocatechol (Catechol) by Monomethylation with Potassium methyl sulfite, or with Dimethylsulfate in aqueous alkali.

4-57; 31-146; 26-596; 68-467; 85-67; 86-56; 90-376; 100-499; 160-1022; B-VI-768;

## 1473: GUAIACOL ALLYLETHER

Catechol methylallylether.

NOTE: There is considerable risk of confusing this name with the names of the following Aroma-chemicals:
*para*-Allylguaiacol = Eugenol.
5-Allyl guaiacol = Chavibetol.



$C_{10}H_{12}O_2 = 164.21$

Pale yellowish or almost colorless viscous oil.

Insoluble in water, soluble in alcohol and oils.

Dry-peppery, rather choking and green odor with slightly fatty and remotely fruity notes.

Sweet, but burning taste with a somewhat medicinal nuance.

This Phenolether which was developed in search of perfume and flavor materials other than the conventional members of the Eugenol family, has never achieved much popularity, even when it was freely available some 10 years ago. It could find some application in heavier floral fragrances, perhaps trace amounts in Carnation and Wallflower bases, variations of Rose fragrances, etc.

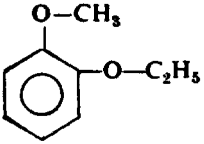
To the author's knowledge, this material is not used in flavor compositions.

Prod.:
1) from Pyrocatechol by treatment with Allyl bromide in Acetone in the presence of Potassium carbonate under cooling, followed by Methylation with Dimethylsulfate in aqueous alkali.
2) from Guaiacol by reaction with Allylbromide.

See also: 68-468;

## 1474: GUAIACOL ETHYLETHER

*ortho*-Ethoxy anisole.
Catechol methylethylether.
*1*-Methoxy-*2*-ethoxy benzene.



$C_9H_{12}O_2 = 152.20$

Colorless or pale straw-colored oily liquid. B.P. 213° C.

Almost insoluble in water, soluble in alcohol, miscible with oils. Poorly soluble in Propylene glycol.

Very sweet, earthy-herbaceous, somewhat musty-walnut-like odor of fair tenacity. The few variations of samples show occasional contamination with traces of Phenol, which largely disturbs the odor of the ether.

This "mixed" ether, which is rarely offered commercially, could find some use in perfume formulations as a modifier for Coumarin or Hydroquinone dimethylether. It is somewhat more medicinal than these, does not have the anisic sweetness or pronounced nutlike pungency of the related materials. It is much less tenacious, and this may be one reason why it has never become very popular.

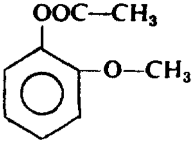
Prod.: by Ethylation of Guaiacol with Diethyl sulfate in aqueous alkaline solution.

68-467;

## 1475: GUAIACYL ACETATE

Acetyl guaiacol.
*1*-Acetoxy-*2*-methoxy benzene.
*ortho*-Methoxy phenylacetate.

NOTE: It is most conceivable that this material is often confused with Guaiyl acetate (Guaiacwood acetate). The latter is much more common in perfumery.



$C_9H_{10}O_3 = 166.18$

Almost colorless or pale straw-colored oily liquid. Sp.Gr. 1.16. B.P. 241° C.

Very slightly soluble in water, soluble in alcohol and oils.

Woody, dry, slightly green odor with variable amounts of a medicinal note, according to purity of the chemical. Overall rather uninteresting, and it is the author's belief, that this Acetate has entered the perfumery literature by accident rather than by merit of fragrance.

Although the immediate impression is that of more power than Guaiyl acetate, the odor of Guaiacyl acetate is actually weak and does not offer any interesting effect to the perfumer.

It is used (according to confirmed information) in flavor compositions, e. g. in Berry complexes at the rate of about 3 to 15 ppm in the finished consumer product. The author agrees that this Acetate could possibly find use in Blackcurrant and similar flavors.

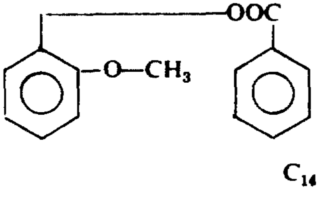
G.R.A.S.

Prod.: by Acetylation of Guaiacol with Acetic anhydride in an inert solvent.

26-566; 90-377; B-VI-774;

## 1476: GUAIACYL BENZOATE

"Benzosol".
Benzoyl guaiacol.
*ortho*-Methoxy phenylbenzoate.



$C_{14}H_{12}O_3 = 228.25$

Colorless crystalline powder. M.P. 58° C. Almost insoluble in water. Poorly soluble in cold alcohol, soluble in hot alcohol, miscible with oils.

Virtually odorless when pure and freshly prepared.

Very faint taste, rather nondescript, sweet-balsamic, woody.

Apart from being a possible fixative of rather poor value, this material can hardly offer any interesting effects to the creative perfumer or to the flavorist.

It is mentioned partly because of possible confusion with the esters of Guaiol.

Prod.: from Guaiacol in aqueous alkaline solution with Benzoyl chloride.

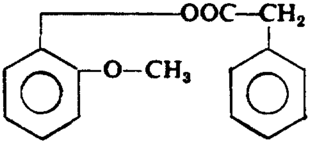
17-63; 26-566; 100-500; B-IX-130;

## 1477: GUAIACYL PHENYLACETATE

*ortho*-Methoxy phenol phenylacetate.

NOTE: Do not confuse with: Guaiyl phenylacetate, which is a chemical with possible application in perfumery and in food flavors. The subject chemical is most conceivably the result of an old typographical error or chemical misunderstanding, since it has very little, if any, perfumery interest.

It is very likely that this phenylacetate was produced in the attempt to make *Guaiyl* phenylacetate, a chemical based upon two raw materials, both of interest to the perfumer for Rose type fragrances. However, Guaiacol will not produce esters or ethers of that type, and the Phenylacetate in particular, is certainly not a floral fragrance material.



$C_{15}H_{14}O_3 = 242.28$

Usually an amber-colored viscous liquid, solidifying in the cold. When pure, it forms colorless crystals, melting to an almost colorless liquid.

Heavy, rather dry, woody-herbaceous odor with variable amounts of "phenolic" or "phenylacetic" notes, both of which will greatly influence the odor of the ester.

The author believes that this material is rarely, if ever, used in perfume compositions.

It finds some use in flavor compositions for imitation Coffee, Honey, Tobacco, and in Berry complexes. It is also used in the creation of smokey flavor bases for meat and fish products.

The concentration used is equivalent to about 0.4 to 3 ppm in the finished consumer products.

G.R.A.S. F.E.M.A. No.2535.

Prod.: from Phenylacetyl chloride and Guaiacol in aqueous alkaline solution, or in Pyridine solution.

## 1478: GUAIENE

Mainly: *1,4*-Dimethyl-*7*-*iso*-propenyl-*Δ9,10*-octahydroazulene, and related hydrocarbons.

NOTE: Do not confuse with *2,3*-Dimethylnaphthalene, which was formerly called Guaiene.

$C_{15}H_{24} = 204.36$

The commercial product is a mixture of hydrocarbons obtained from Guaiol, the sesquiterpene alcohol which forms chief constituent of Guaiacwood oil. The alcohol is dehydrated to Guaiene.

Guaiene is an almost colorless oily liquid.

Insoluble in water, soluble in alcohol, poorly soluble in diluted alcohol. Miscible with most perfume oils.

Pleasant sweet-woody, mild and almost balsamic odor with a discrete peppery undertone and good tenacity.

The use of Guaiene has been suggested since it offers a variation of the conventional

Guaiacwood odor, which unfortunately too often is accompanied by a "smoked ham"-like odor, conceivably acquired during forced distillation of the Guaiacwood in adding mineral acid to the distillation water in order to increase yield and speed of distillation.

Guaiene is therefore more versatile than Guaiacwood as a fragrance material, and it may also be used as a modifier for Vetiver- or Cedarwood-products in woody or non-floral-aldehydic fragrance types, as well as in woody or Oriental ones. It blends well with Oakmoss products, Olibanum, Lavender, and Lavandin, Ambrematerials, etc.

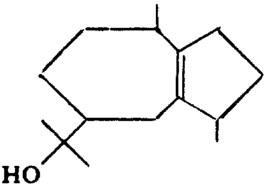
Guaiene has also served as basis for the making of artificial Patchouli oil during the period (1965-67) of exceptionally high prices for the natural oil.

Approved for food flavor use by the F.R.

68-1285; 87-281; (sample from Fritzsche Bros. Co.).

## 1479: GUAIOL

A sesquiterpenoid alcohol.
*1,4*-Dimethyl-*7*-(*alpha*-hydroxy-*iso*-propyl)-$\Delta^{9,10}$-octahydroazulene.



$C_{15}H_{26}O = 222.37$

Colorless prismatic crystals. M.P. 93° C. B.P. 263° C. Sp.Gr. 0.91 (liquid).

Insoluble in water, soluble in alcohol, miscible with perfume oils.

Deteriorates when exposed to air, becomes semi-liquid, darkens in color and changes odor.

Mild, rather sweet and very tenacious balsamic-woody odor with an almost floral undertone and a pepperiness which seem to be apparent only in impure material (possibly traces of hydrocarbons).

Guaiol as such is not often used in perfumery. It could provide a suitable basis for many woody and floral-woody complexes, since it blends excellently with floral odors as well as naturally with all types of woody odors. It could form an excellent basis for Carnation and a pleasant background in a Chypre or modern woody-aldehydic fragrance.

A few – chemically impure – esters of Guaiol are used more widely in perfumery and occasionally in flavors.

Apart from its strange sensitivity to air (Oxygen), Guaiol seems to be very resistant to most of the conventional reactants with which derivatives are normally made.

Prod.: by extraction from Guaiacwood oil with a volatile solvent, usually Acetone, Ethanol or Ethylether.

It can also be isolated from the wood of certain Australian members of the family Taxodiaceae, particularly the so-called "Murray River Pine".

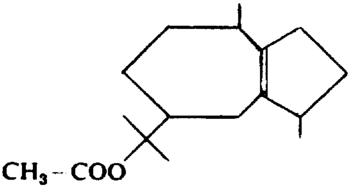
7-200; 4-57; 67-666; 88-284;

## 1480: GUAIYL ACETATE

"Guaiacwood acetate".
*1,4*-Dimethyl-*7*-(*alpha*-hydroxy-*iso*-propyl)-$\Delta^{9,10}$-octahydroazulene acetate.

This commercial product contains significant amounts of Guaiol and other non-acetylated products.

"Madrysia" (Firmenich), is mainly Guaiyl acetate.



$C_{17}H_{28}O_2 = 264.41$

Pale yellowish or almost colorless viscous liquid. Sp.Gr. 0.99. B.P. approximately 269° C.

Insoluble in water, soluble in alcohol and oils.

Delicately sweet-woody, soft and warm odor reminiscent of Patchouli and Tearose. There will normally be undertones of Guaiacwood-like character, but the absence of such notes is appreciated by most observers who prefer the acetate for its clean, floral-woody and sweet tenacity. The total absence of "smoked-ham" notes is of imperative significance to the beauty of the odor of Guaiyl acetate.

This ester is used in perfume compositions of the more delicate types, such as Crepe de Chine or certain variations of Rose, but it finds application in many woody fragrances, Chypres and Men's fragrances, etc. It can, to a certain degree, substitute for Vetiveryl acetate in many types of modern fragrance, although in higher concentration it does show a significant lack of sweetness as compared to the Vetiver derivative. It is very interesting in Carnation bases, and it provides good fixation for powder perfumes.

Guaiyl acetate is used in Tobacco and fruit flavors in minute traces, usually only 0.5 to 2 ppm in the finished product. It gives a useful and interesting background in Blackcurrant, Peach, Apricot, Strawberry and even Pineapple, etc.

Prod.: by Acetylation of Guaiacwood or the isolated sesquiterpene fraction (Guaiol) of same. Acetylation of pure, extracted Guaiol does not even yield a pure Acetate. High-grade commercial esters may have nearly 90% ester content, calculated as Guaiyl acetate.

G.R.A.S.

4-57; 33-516; 17-200; 106-181;
See also monograph: Guaiacyl acetate.

## 1481: GUAIYL BUTYRATE

The *n*-Butyric acid ester of the sesquiterpene alcohols isolated from Guaiacwood oil.
Structure: see Guaiyl acetate.

$C_{15}H_{25}$—$OOC(CH_2)_2CH_3$

$C_{19}H_{32}O_2 = 292.47$

Pale yellowish or almost colorless viscous oil. Sp.Gr. 0.99. B.P. approximately 277° C.

Insoluble in water, soluble in alcohol and oils.

Very mild, sweet-woody-floral odor with distinctly animal undertones.

This odor type is very suitable for certain variations of Rose, where Civet or Honey-notes are called for, and in Oriental Rose variations in combination with heavy woody and floral notes.

The ester is very far from pure, normally about 80% ester content, and a certain amount of purely woody notes must be expected.

The ester has found a little use in artificial Patchouli oil.

In flavors it could be used for the very heavy fruity types, such as Fig and Date, two flavors which are difficult to reproduce from pure chemicals.

Prod.: from the extracted Guaiacol from Guaiacwood oil by treatment with Butyric anhydride.

4-57; 33-734; 86-56;

## 1482: GUAIYL FORMATE

The formylated sesquiterpenealcohol fraction of Guaiacwood oil.
Structure: see Guaiyl acetate.

$C_{15}H_{25}$—$OOCH$

$C_{16}H_{26}O_2 = 250.38$

Pale yellowish oily liquid. Sp.Gr. 1.00.

Insoluble in water, soluble in alcohol and oils.

Peculiar green-woody, yet somewhat floral and tenacious odor with bark- or sap-like undertones.

The formate is normally very far from chemically pure, about 65 to 75% ester content in the commercial product.

The odor depends therefore to a large degree upon the quality of the balance of the material.

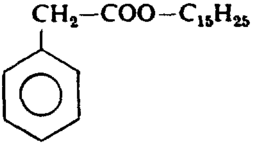
This ester is very rarely offered commercially, and the author believes that it is only very occasionally used in perfumes. It could probably act as a modifier for Guaiacwood oil or for the isolated Guaiol in modern aldehydic-woody fragrance types. It gives very interesting effects with purified Galbanum products.

Prod.: from isolated Guaiol by Formylation with Formic acid and Acetic anhydride.

4-57;

## 1483: GUAIYL PHENYLACETATE

The phenylacetic acid ester of the sesquiterpene alcohol Guaiol, isolated from Guaiacwood oil.
Structure: see Guaiyl acetate.



$C_{23}H_{32}O_2 = 340.51$

Colorless crystals or pale yellowish crystalline mass, or viscous, yellowish liquid. The crystals melt at approximately 38° C. The liquid may remain supercooled for a long time without solidifying. Sp.Gr. 1.01. B.P. well over 300° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, but delicately sweet and mildly woody-floral odor of outstanding tenacity. This material is perfectly made for fixation of heavy florals, and as a base in delicate or very sweet floral types, such as Honeysuckle and Frangipanni. It gives interesting effects with the conventional carbinols in Lilac, and it lends a fine background in Honey bases for perfumes.

This ester could find some use in flavor compositions, particularly in imitation Honey, and in Tobacco flavors.

It is most conceivable that this is the ester originally desired by the perfumers, when various Phenylacetates became commercially available. The thought that a combination of the woody Rose notes from Guaiacwood could be combined with the heavy animal sweetness of Phenylacetic acid in an ester, is obvious to the perfumer's mind.

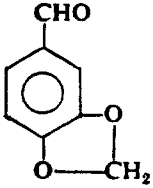
However, many literature references are unfortunately referring to *Guaiacyl* phenylacetate in this connection. See that monograph for further comments.

Prod.: from Guaiol isolated from Guaiacwood oil by reaction with Phenylacetyl chloride in an inert solvent.

7-200; 34-248; 4-57; 86-56;
NOTE: several of these literature references may actually be based upon *Guaiacyl* ester.

## 1484: HELIOTROPINE

Dioxymethylene protocatechuic aldehyde.
Protocatechualdehyde methylene ether.
*3,4*-Methylene dioxybenzaldehyde.
Piperonyl aldehyde.
Piperonal.



$C_8H_6O_3 = 150.14$

White or colorless crystals. M.P. 37° C. B.P. 263° C.

0.2% soluble in cold water, somewhat better in hot water. Soluble in alcohol and oils, somewhat soluble in Propylene glycol. Insoluble in Glycerin. Volatile with steam.

Very sweet floral, warm slightly spicy and tenacious odor, sometimes described as "Cherry-like" (American type Cherry).

Sweet, spicy-floral taste of considerable power.

The "spicy" notes should not reveal a Safrole-like character, but rather indicate a warm, almost herbaceous-fruity note similar to that in Benzaldehyde, Anisaldehyde, Anisylacetate, etc. The floral note in Heliotropine is very sensitive to the presence of Safrole-like impurities.

The taste is slightly bitter at concentrations higher than 50 ppm.

Heliotropine is very extensively used in perfume compositions – from the very expensive types all the way down to household fragrances and industrial perfumes. Concentrations may vary from less than one percent to more than ten percent, but floral effects are usually obtained with a few percent. The presence of Heliotropine at lower concentrations is normally revealed in the "dryout" of the perfume on a blotter, while higher concentrations may show Heliotropine conspicuously in the topnote too. Althought primarily a floral ingredient, it blends very well with many nonfloral materials, such as the Coumarins, the Eugenols, Nitromusks, Cedarwood derivatives, etc.

It is almost a "must" in Lilac and Sweet Pea, and it is often used in Muguet, Honeysuckle, Frangipanni, Carnation, Mimosa, etc.

Contrary to earlier belief and repeated statements, Heliotropine is not necessarily a problem in a soap perfume. Today's high-quality re-crystallized Heliotropine is virtually free from impurities which, according to general belief, have been responsible for most of the discoloration in soap – directly or indirectly (catalytically perhaps). The quality of soap today is furthermore of such standard that it causes less problems with respect to alkalinity and foreign metals or other chemically active matter. Discoloration problems from soap perfumes containing Heliotropine are, accordingly, rarely due to the Heliotropine alone, but may be due to an accentuated problem from several perfume ingredients, including or not including Heliotropine.

Heliotropine is, however, very sensitive to certain Amines, e. g. Indole. The vapors emanating from an Indole container may penetrate the walls of a Heliotropine container and color its content pink. Such contamination can take place over a considerable distance and should be considered when storing these materials. Today's polyethylenelined fiberpaks do NOT protect against such damage.

Heliotropine finds extensive use in flavor compositions, although the power of Heliotropine as a flavoring agent is often underestimated, and the concentration should be kept at a minimum in order to achieve truly pleasant and "non-perfumey" effects.

The most interesting effect of Heliotropine as a flavor material is probably that of being a synergist to Vanillin, and not in quite the same way as Coumarin has been. It gives a considerable "lift" to an imitation Vanilla flavor, but the amount of Heliotropine in proportion to Vanillin/Ethylvanillin must be kept very low.

Another interesting effect of Heliotropine is that of giving a "Cherry-pit"-like effect in fruity complexes or in Cherry imitation flavor. It is a pleasant deviation from the harsh Benzaldehyde, so conventionally used in American so-called Cherry flavor, and it adds richness to an imitation flavor which may be high in volatile esters. It blends excellently with Anisalcohol and its esters in Vanilla, Peach and Plum, and in variations of the Cherry flavor.

It is also used in Strawberry, Cola, Rum, Maple, Nut and "Tutti-frutti" flavors.

The concentration used is normally about 5 to 20 ppm in the finished product, except in Chewing gum up to 40 ppm.

Prod.:

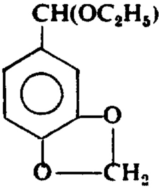
1) by oxidation of *iso*-Safrole. The latter is obtained by isomerization of Safrole, a distillation (or freezing) isolate from Brazilian Ocotea pretiosa oil (Ocotea cymbarum) or Chinese Camphor oil ("Sassafrassy fraction").
2) from Catechol (Pyrocatechol).

G.R.A.S. F.E.M.A. No.2911.

4-58; 5-138; 26-660; 1-514; 68-747; 77-207; 72-61; 85-68; 86-56; 90-522; 100-824; 106-183; 156-175; 160-1174; B-XIX-115; 140-164;

## 1485: HELIOTROPINE DIETHYLACETAL

Piperonal diethylacetal.



$C_{12}H_{16}O_4 = 224.26$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils. B.P. 280° C. Sp.Gr. 1.13.

Very mild floral, sweet odor of mildly green-spicy type, remotely reminiscent of Heliotrope and Hawthorne – but much weaker.

The author finds that this material is of very little value and could not possibly arouse much interest among other perfumers even if the material were made commercially available.

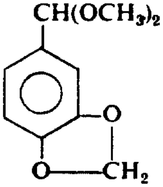
This acetal finds a little use in flavor compositions for its creamy-nut-like taste in imitation Coconut, Nut, Cream, Vanilla, and other flavors, particularly those intended for baked products.

Prod.: from Heliotropine and Ethanol with dehydrating agent.

86-56; 140-164;

## 1486: HELIOTROPINE DIMETHYLACETAL

Piperonal dimethylacetal.



$C_{10}H_{12}O_4 = 196.21$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils. B.P. 273° C. Sp.Gr. 1.21.

Very weak, sweet-floral and somewhat green odor reminiscent of Heliotrope, but much weaker.

Mild, semi-dry herbaceous, Cherry-pit-like taste.

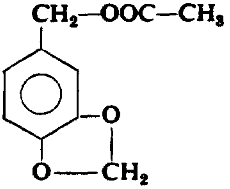
There is hardly more than academic interest in this item. Heliotropine in today's high-purity grade causes very little trouble in soap, and most soaps are not nearly as alkaline as they were 15 or 25 years ago, when the discoloration in soap from use of (impure) Heliotropine was a common problem and caused the chemists to search for more stable derivatives.

Prod.: from Heliotropine and Methanol with a dehydrating agent.

86-56;

## 1487: HELIOTROPYL ACETATE

Piperonyl acetate.
*3,4*-Methylene dioxybenzylacetate.



$C_{10}H_{10}O_4 = 194.19$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet, light, floral and tenacious odor with distinctly fruity ("Cherry-like") undertones.

Sweet, fruity and moderately floral taste, slightly bitter at concentrations above 100 ppm.

This ester finds a little use in finer perfumes, where it may give a delicate sweetness and powdery notes to Cassie bases, Muguet and Lilac fragrances, Magnolia and other delicate florals. It is comparatively expensive, and its cost is prohibitive for its wider use. Besides, its effects are not absolutely unique, and many perfume laboratories have probably never had this item on the shelf.

In fruit-flavors it reveals fruity notes more than floral ones, and it is also weaker than Heliotropine as a flavor material. Traces may be used as modifier for the Anisyl derivatives in Vanilla imitation. The ester is quite useful in "Tutti-frutti" type of flavor, one of the most popular types of flavor next to the Mint flavors in chewing gum.

Concentration is normally about 25 to 80 ppm in the finished product.

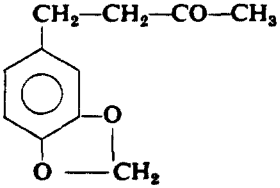
Prod.: by esterification of Heliotropyl alcohol with Acetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2912.

86-117;

## 1488: HELIOTROPYL ACETONE

Piperonyl acetone.
*3,4*-Methylene dioxybenzyl acetone.
*4*(*3,4*-Methylenedioxyphenyl)-*2*-butanone.
"Cassione" (Firmenich).
"Dulcinyl" (I.F.F.).
"Cyclozingerone" (somewhat confusing name).
"Heliotrope blanc" (a solution of H.A.).



$C_{11}H_{12}O_3 = 192.22$

Colorless crystals or white crystalline granular material.

Impure crystals may be straw-colored.

M.P.55° C. (A lower melting point is observed for certain specialties usually because of the presence of trace additives for "bouquetting".)

Practically insoluble in water, soluble in alcohol, miscible with most perfume and flavor oils.

Intensely sweet, floral and very slightly woody-powdery odor reminiscent of the sweet-floral notes in Mimosa and Cassie. Also remotely reminiscent of Heliotrope.

The taste in dilutions below 50 ppm is sweet, somewhat fruity and "Cherry-pit"-like. Higher concentrations tend to show a somewhat bitter taste.

For several decades well kept as a "secret" chemical this ketone is one of the most interesting and successful condensation products from a perfumery point of view. It finds application in Lilac, Lily, Sweet Pea, Appleblossom, Mimosa, Cassie, Ylang-Ylang, Heliotrope, Carnation, etc. and is particularly interesting in lipstick perfumes, also because it blends well with Ionones.

Heliotropyl acetone finds use in flavor compositions for imitation Cherry ("pit flavor") in various fruit complexes. Occasionally as a modifier in Vanilla imitation.

The concentration is about 8 to 45 ppm in finished products. The highest figures are usually in icecream, about 50 ppm.

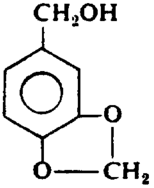
G.R.A.S. F.E.M.A. No.2701.

Prod.: by condensation of Heliotropine with Acetone, followed by hydrogenation in presence of a Palladium catalyst. The Acetone condensation takes place in aqueous alkaline solution.

159-306; 7-203; 7-348; 31-84; 68-990; 90-526; 103-273; there is some confusion in the literature on the subjects: Heliotropylidene Acetone and Heliotropyl acetone. The latter is often described as having a "strong, sharp, peppery, chemical odor", a description which seems to refer to another chemical, probably Methystione, the unsaturated condensation product.

## 1489: HELIOTROPYL ALCOHOL

Piperonyl alcohol.
*3,4*-Methylenedioxy benzylalcohol.



$C_8H_8O_3 = 152.15$

Crystal needles, colorless or white.
M.P. 53° C.

Slightly soluble in hot water, soluble in alcohol, miscible with most perfume oils.

Weak, sweet, nondescript odor, remotely reminiscent of Vanilla.

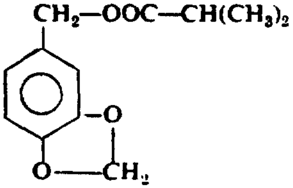
The alcohol as such, has probably very little value as a perfume or flavor material. Certain esters are used to some extent but the author finds that there is rarely, if ever, a definite need for Heliotropyl alcohol in a perfume of a flavor.

Prod.: from Heliotropine by reduction with Sodium amalgam in alcohol.

4-120; 26-660; 86-117; 90-525; B-XIX-67;

## 1490: HELIOTROPYL-iso-BUTYRATE

Piperonyl-*iso*-butyrate.



$C_{12}H_{14}O_4 = 222.24$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Deep-sweet, very mild, overall fruity, berry-like odor with a "jam-like" and a trace of a floral undertone.

Needless to add that mere traces of free *iso*-Butyric acid will heavily influence – and usually destroy – this odor picture.

The flavor is intensely sweet, fruity/fruit-preserve-like, reminiscent of dried plums.

The author is not aware of the use of this ester in perfumery.

It is used to a modest extent in flavor compositions, e. g. imitation Peach, Plum, etc. and in fruit complexes, berry flavors, cheese flavors etc.

The concentration is normally very low, e. g. 0.05 to 3.50 ppm in the finished product.

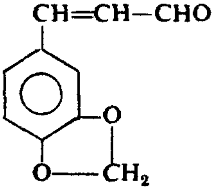
G.R.A.S. F.E.M.A. No.2913.

Prod.: by esterification of Heliotropyl alcohol with *iso*-Butyric acid under azeotropic conditions.

86-117;

## 1491: HELIOTROPYLIDENE ACETALDEHYDE

Piperonylidene acetaldehyde.
Piperonyl acrolein.
*3,4*-Methylenedioxycinnamic aldehyde.



$C_{10}H_8O_3 = 176.17$

White crystalline material. M.P. 86° C.

Very slightly soluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Sweet-balsamic and very tenacious odor. The floral notes which could be expected, are hard to find, and the power is much inferior to that of Heliotropine. However, its mild and delicate sweetness is quite attractive, and its tenacity excellent.

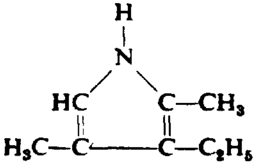
This aldehyde has found some use in perfume compositions partly as a modifier for Heliotropine, partly as component of Cassie bases, once a fragrance type of extraordinary popularity.

Prod.: from Heliotropine and Acetaldehyde by condensation in weak aqueous alkali.

68-986; 90-534;

## 1492: iso-HEMOPYRROLE

Cryptopyrrole.
*3*-Ethyl-*2,4*-dimethyl pyrrole.



$C_8H_{13}N = 123.24$

Colorless mobile liquid. B.P. 182° C.

Solidifies in the cold, melts again at 17° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and rather pungent, but sweet, somewhat floral odor, rather choking at high concentration, warm-exotic, floral at proper dilution.

The use of this material has been suggested since many Pyridine derivatives had enjoyed a success as trace ingredients in certain floral fragrance types (Jasmin, Tuberose, Gardenia, etc.).

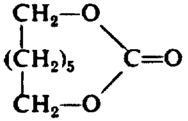
However, this material is very rarely offered commercially by the regular producers of perfume chemicals, and it is comparatively unknown as a fragrance material. There are still discussions as to the safety of using these materials in cosmetic preparations, although the concentrations generally applied are in the order of magnitude of one ppm in the functional product. (See also Piperidine).

Prod.:

1) from Pyrrole by Grignard type Alkylation.
2) by reduction of Chlorophyll derivatives with Hydriodic acid, followed by separation of the homologues and isomers formed.

1-776; 69-44;

## 1493: HEPTAMETHYLENE CARBONATE



$C_8H_{14}O_3 = 158.20$

White or colorless crystals. Insoluble in water, soluble in alcohol and oils.

Faint camphoraceous-minty odor, remotely reminiscent of Pennyroyal oil or Pulegone, yet slightly more medicinal-tarry.

In the author's opinion, this material has no interest to the creative perfumer beyond some academic interest or a possible use as an odorant for industrial masking.

Prod.: from Heptylene glycol with Carbonyl chloride.

31-127;

## 1494: n-HEPTANAL

Enanthal.
Oenanthal.
Enanthaldehyde.
Oenanthic aldehyde.
"Oenanthol" (misleading name).
Aldehyde C-7.
Heptanoic aldehyde.
*n*-Heptyl aldehyde.
Heptaldehyde.

$CH_3(CH_2)_5—CHO$

$C_7H_{14}O = 114.19$

Colorless oily, yet mobile liquid.
Sp.Gr. 0.82. B.P. 153° C.

Slightly soluble in water, miscible with alcohol and oils.

Very powerful and diffusive oily-fatty, "rancid" odor. Penetrating and pungent at high concentration, almost fruity, "fermented-fruit"-like in extreme dilution.

Harsh, fatty-rancid taste in high concentration, but becomes sweet Almond-like, nut-like and nondescript fruity in dilutions below 1 ppm.

The aldehyde finds some use in perfumery, mostly for masking odors for industrial purposes, also in a few special fragrance types. Minute traces can have interesting effect upon floral fragrances or artificial flower absolutes, essential oils, etc.

The aldehyde is used in very discrete amounts in imitation Apple, Ginger, Citrus, Cognac, Almond, Melon, Rum and Honey flavors. The concentration will normally be about 1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2540.

Prod.: by cracking (destructive distillation) of Castor oil.

4-58; 5-73; 26-566; 31-28; 31-47; 32-60; 34-806; 77-202; 86-56; 89-22; 100-512; 106-32; 101-3; 160-968; B-I-695; 140-158;

## 1495: HEPTANAL DIETHYLACETAL

Heptaldehyde diethylacetal.

$CH_3(CH_2)_5CH(OC_2H_5)_2$

$C_{11}H_{24}O_2 = 188.31$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. B.P. 204° C. Sp.Gr. 0.84.

Fresh-herbaceous, winey and foliage-green odor, sweeter and much less penetrating than that of the aldehyde.

This Acetal has been suggested for use in Jasmin bases to introduce the winey-green note that forms part of the very complex topnote of Jasmin.

It is occasionally used in flavor compositions for imitation Lemon, Brandy, Cognac, etc., normally in mere traces.

Prod.: from Heptaldehyde and Ethylalcohol with a dehydrating agent. Another method uses Heptaldehyde plus Formiminoethylether hydrochloride.

5-318; 35-58; 86-57;

## 1496: HEPTANAL DIMETHYLACETAL

Heptaldehyde dimethylacetal.

$CH_3(CH_2)_5CH(OCH_3)_2$

$C_9H_{20}O_2 = 160.26$

Colorless liquid. B.P. 180° C. Sp.Gr. 0.85.

Very slightly soluble in water, soluble in alcohol and oils.

Green-herbaceous, vegetable-like odor, reminiscent of green beans (haricots verts), almost cabbage-leafy, with sweet-oily, somewhat coconut-like undertones.

It is interesting to note the repeatedly appearing "coconut-note" in alifatic chemicals with 9 Carbon atoms, Alcohols, Aldehydes, Ketones, Esters, Acetals, etc.

Peculiar green-vegetable taste with a nuance of fungus-like taste.

The use of this acetal in Jasmin bases has been suggested. It could undoubtedly be used as part of the topnote complex in many fragrance types, not only the floral and fruity ones. In Fougère types, rich in herbaceous notes, it can give quite interesting effects with or without the support of Oakmoss.

The Acetal is used in minute amounts in imitation fruit flavors, e. g. Melon, and in Mushroom flavors, etc.

The concentration is about 0.1 to 1.0 ppm in the finished product.

Prod.: from Heptaldehyde and Methanol with a dehydrating agent.

G.R.A.S. F.E.M.A. No.2541.

5-318; 37-281; 45-58; 84-1; 86-57; 4-58; 140-158;

## 1497: HEPTANAL DI-iso-PROPYLACETAL

Heptaldehyde di *iso*-propyl acetal.

$CH_3(CH_2)_5CH[OCH(CH_3)_2]_2$

$C_{13}H_{28}O_2 = 216.37$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Winey-herbaceous, oily-green odor. Ethereal and mild when pure, but traces of free Aldehyde influences the odor picture considerably to the disadvantage of the Acetal.

In the author's opinion, only the cyclic Acetals of Heptaldehyde are of considerable interest, being powerful and distinctly different in odor type from their parent Aldehyde. The Acetals with Ethylene- and Propylene glycol are both interesting and well known (under trade names).

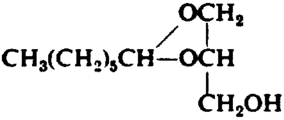
Prod.: by condensation of *n*-Heptanal and *iso*-Propylalcohol. The Acetal is formed spontaneously.

31-67;

## 1498: HEPTANAL GLYCERYL ACETAL

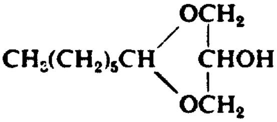
The commercial product is a mixture of the Acetals in the *1,2*- and *1,3*-position:
A: *2*-Hexyl-*4*-hydroxymethyl-*1,3*-dioxolan,
and:
B: *2*-Hexyl-*4*-hydroxy-*1,3*-dioxan:

A:



and

B:



$C_{10}H_{20}O_3 = 188.28$

Colorless viscous liquid. Very slightly soluble in water, soluble in alcohol and oils.

Peculiar fungus-like, earthy-sweet odor, not very powerful.

Sweet Mushroom (Champignon)-like taste in proper dilution.

Beyond some possible use in a few rare cases (Hyacinth, etc.), this Acetal is hardly ever used in perfumery.

It finds some use in flavor compositions for imitation Mushroom.

The concentration used is about 5 to 100 ppm in the finished product.

Prod.: by condensation of Heptaldehyde with Glycerin.

G.R.A.S. F.E.M.A. No.2542.

5-322; 84-1;

## 1499: HEPTANE

*n*-Heptane.

$CH_3(CH_2)_5CH_3$

$C_7H_{16} = 100.21$

Colorless mobile liquid. Sp.Gr. 0.68.
B.P. 98° C.
Almost insoluble in water, soluble in alcohol (up to equal parts) miscible with most oils.

Sweet-ethereal, diffusive odor of poor tenacity. Commercial grade material often carries off-odor of sulfuraceous, tarry, phenolic or "gassy" Styrene-like character, deriving from trace impurities, while pure Heptane is not unpleasant smelling at all.

Although this hydrocarbon cannot be classified as a perfume or flavor material, it may occur as a trace component in perfume and flavor raw materials, extracted from natural materials using e. g. Heptane as a solvent. Flower absolutes or spice oleoresins, etc. can carry the hydrocarbon, and the title material has therefore been included in the F.E.M.A. list as G.R.A.S. Accordingly it may be used as a "synthetic flavoring adjuvant".

Heptane is flammable and its vapors form explosive mixtures with air at room temperature.

Prod.: by isolation from Petroleum. Heptane is a component of the light fraction known as gasoline.

26-566; 66-247; 100-512; 160-1026; B-I-154;

## 1500: HEPTANOIC ACID

Enanthic acid.
Oenanthic acid.
*n*-Heptylic acid.
*n*-Heptoic acid.

$CH_3(CH_2)_5COOH$

$C_7H_{14}O_2 = 130.19$

Colorless oily liquid. Solidifies in the cold, melts at minus 8° C. B.P. 223° C.
Sp.Gr. 0.92.

0.3% soluble in cold water, soluble in alcohol, miscible with oils.

The commercial product has a very unpleasant, sour-sweat-like, fatty odor. A highly purified acid is considerably more attractive, although it still has a fatty odor, it is more fat-like without having the typical "rancid" odor or sweat-like notes.

Traces of this acid are occasionally used in perfume compositions, e. g. in Labdanum compositions and in artificial Civet.

Prod.: by oxidation of Heptaldehyde.

7-208; 26-566; 100-512; 160-968; B-II-338; 140-141;

## 1501: 1-HEPTANOL

*n*-Heptanol-*1*.
*n-primary*-Heptylalcohol.
Hexyl carbinol.
*1*-Hydroxyheptane.
Enanthyl alcohol.
Alcohol C-7.
Enanthic alcohol.

$CH_3(CH_2)_5—CH_2OH$

$C_7H_{16}O = 116.21$

Colorless oily liquid. 0.2% soluble in water, soluble in alcohol, miscible with oils.
Sp.Gr. 0.82. B.P. 175° C.

Fresh and light, green-fatty, winey and sap-like odor of poor tenacity.

Sweet winey-nut-like taste. Green only in high concentration.

This alcohol is used in perfume compositions in trace amounts for refreshing effects and lift to Carnation, exotic florals, Oriental bases. Opopanax, Jasmin, etc.

It is also used in flavor compositions for imitation Coconut, and in various fruit complexes.

The concentration used is normally very low, about 1 to 5 ppm in the finished product.

Prod.:
1) by catalytic reduction of Heptaldehyde (from Castor oil).
2) from Ethylene oxide and Pentane with Aluminium bromide catalyst.

G.R.A.S. F.E.M.A. No.2548.

4-58; 26-568; 31-15; 31-21; 66-313; 77-171; 86-57; 87-468; 100-512; 106-25; 160-1028; B-I-414; 140-124;

## 1502: 2-HEPTANOL

*2*-Hydroxyheptane.
*n*-Heptanol-*2*.
*secondary*-Heptylalcohol.
Methyl amyl carbinol.
Exists in *laevo-*, *dextro-* and *d,l*(*racemic-*, most common form) isomers.

$CH_3-\underset{\underset{OH}{|}}{C}H(CH_2)_4CH_3$

$C_7H_{16}O = 116.21$

Colorless liquid. Sp.Gr. 0.82. B.P. 158° C.

0.4% soluble in water, soluble in alcohol and oils.

Fresh, Lemon-like, grassy-herbaceous odor with a sweet-floral undertone. The overall "lift" is primarily fruity-green.

Fruity and somewhat green, but also rather bitter taste.

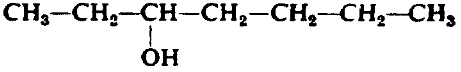
This alcohol finds a little use in perfume compositions, particularly in the reproduction of certain essential oils, e. g. Clove and Cinnamon. It is occasionally used as part of a herbaceous-green topnote theme for novel versions of Fougere or "forest" bases, etc., and in various places where a refreshing topnote of non-floral character is desirable.

Prod.: from Amylmagnesium bromide and Acetaldehyde. It can also be produced by catalytic reduction of Methyl amyl ketone.

4-59; 26-568; 45-60; 87-469; 100-512; 160-1028; B-I-415; 4-87; 7-136; 7-269;

## 1503: 3-HEPTANOL

Ethyl butyl carbinol.
*n*-Butyl ethyl carbinol.



$$CH_3-CH_2-\underset{OH}{\underset{|}{CH}}-CH_2-CH_2-CH_2-CH_3$$

$C_7H_{16}O = 116.21$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful, herbaceous, warm-and-cool odor of poor tenacity. In dilution sweet, more balsamic than herbaceous.

Pungent, slightly bitter taste in concentrations higher than 30 ppm.

This alcohol, only recently made commercially available through the conventional sources of perfume and flavor raw materials, has been suggested for use as a trace component in various artificial essential oils.

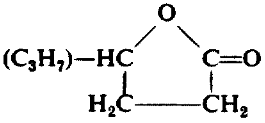
It is also used in minute amounts in various flavor compositions, since related materials have been identified in many food products, including bread (at the dough stage).

Prod.: by catalytic hydrogenation of Ethyl-*n*-butyl ketone. The latter is obtained either by acetylenic hydrolysis or via substituted Ethylene oxide.

Approved for food flavor use (U.S. Federal Register 1965).

## 1504: HEPTANOLIDE-(4,1)

*gamma-n*-Propyl-*gamma*-butyrolactone.
*gamma*-Heptalactone.



$C_7H_{12}O_2 = 128.17$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol, miscible with oils.

Sweet-herbaceous, nut-like and slightly caramellic odor, practically free from fatty notes. Moderate tenacity.

Somewhat malty-caramellic, sweet-herbaceous and nut-like taste, reminiscent of those of Coumarin and Dihydrocoumarin, often described as "tobacco-like" (probably meaning "tobacco-flavor-like").

This lactone has been suggested for use in perfumes, but it has not achieved much popularity for such purpose. It resembles Coumarin very much in effect, and it carries similar disadvantages in chemical sensitivity and stability. It is general opinion of soap perfumers that Heptalactone does not equal Coumarin as a soap perfume material, and since the subject material is more expensive than Coumarin, it has a hard time getting into regular use in perfumes.

However, in flavors, it has several advantages. It is permitted as a food flavor (Coumarin is not), and it is more versatile than Coumarin, in certain respects also slightly more powerful. It performs well with other crystalline flavor materials and may give synergistic effects toward Vanilla and Coconut combinations. It is used mostly in Nut, Coconut, Vanilla and Caramel or Butterscotch.

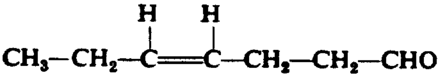
The concentration used is about 20 to 40 ppm in the finished product. The minimum perceptible for Heptalactone alone is about 2 ppm.

G.R.A.S. F.E.M.A. No.2539.
Prod.:
1) by lactonization of Heptenoic acid.
2) by condensation of Methylacrylate and Butylalcohol with a catalyst.
3) via Rothstein's method from substituted Ethylene oxide and Sodio-Malonic ester.

31-172; 156-226;
(sample: Fritzsche Bros. Co.).

## 1505: cis-4-HEPTEN-1-AL

*n*-Propylidene butyraldehyde.



$CH_3-CH_2-CH=CH-CH_2-CH_2-CHO$

$C_7H_{12}O = 112.17$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Extremely powerful, fatty-green, somewhat vegetable odor of moderate tenacity.

When suitably diluted, the odor becomes very "food"-like, reminiscent of the odor of Butter from a frying pan.

The taste is pleasant only in concentrations below 0.1 ppm.

Except for very rare applications in artificial essential oils, this aldehyde is probably not used in perfume compositions.

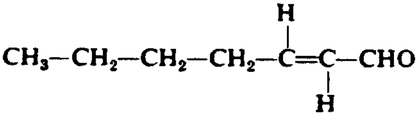
It finds some use in flavor compositions, e. g. in the reconditioning of flavor in fried food, "French fried" potatoes, etc. The effect in extreme dilution simulates the flavor of Cream to a certain extent.

The aldehyde is present in Butter at the concentration of 0.0015 ppm.

(Sample: Compagnie Parento, Inc. U.S.A.).
157-315; 158-95;
see also: 156-25;

## 1506: trans-2-HEPTEN-1-AL

*alpha-beta*-Heptenoic aldehyde.
*beta*-Butyl acrolein.
*2*-Heptenal.



$CH_3-CH_2-CH_2-CH_2-CH=CH-CHO$

$C_7H_{12}O = 112.17$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 159° C.

Almost insoluble in water, soluble in alcohol, miscible with oils.

Pungent-green odor, only in extreme dilution becoming pleasant, vegetable-juicy-green, but more fatty than the Hexenoic aldehydes.

This aldehyde, not nearly as popular as the Hexenoic series, has been suggested for use in perfumes (and flavors).

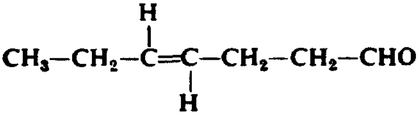
It can be used in the reconstruction of Galbanum (oil) notes, or – separately – in minute amounts to accompany Geranium or fruity-floral topnote complexes, fruity-herbaceous notes, etc. It is somewhat more difficult to use than the Hexenal.

Prod.: (several methods, e. g.):
1) by condensation of Acetaldehyde with *n*-Valeric aldehyde.
2) by reduction of *2*-Heptenoic acid with Formic acid vapors over Manganous oxide at 350° C.
3) by oxidation of *2*-Hepten-*1*-ol.

89-42; 156-26;

## 1507: trans-4-HEPTENAL

*trans-n*-Propylidene butyraldehyde.



$$CH_3-CH_2-\overset{H}{C}=\underset{H}{C}-CH_2-CH_2-CHO$$

$C_7H_{12}O = 112.17$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

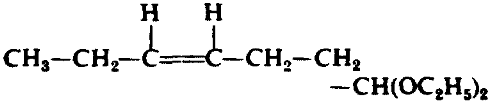
Powerful, fresh-fatty-oily odor, reminiscent of fresh cream.

This rare aldehyde is used in flavor compositions to "reconstitute" the odor of fresh cream - introduce a "creamy" topnote to flavors intended for icecream, whipped cream and many other dairy products.

The concentration normally used in such products is extremely low, about 0.0015 ppm, or 1½ part per 1000 million parts of product.

158-109; 157-303;

## 1508: cis-4-HEPTEN-1-AL DIETHYLACETAL



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-CH(OC_2H_5)_2$$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Comparatively mild and pleasant herbaceous-fruity, "natural" odor. Overall reminiscent of Melon and Apple skins, but with a rich and rather complex herbal undertone.

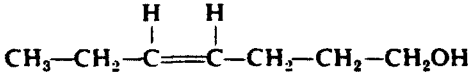
Suggested for use in perfume and flavor compositions. It would undoubtedly find interest among perfumers experimenting with new topnote compositions, Lavender-variations, etc.

Not yet specifically listed as a G.R.A.S. material, it can not be used in flavor compositions in the U.S.A. But it could eventually find some use in Melon flavors, Apple (or "Champagne") flavors, wine flavors for gelatin-candy, etc. where and when it is approved for use in food flavors.

(Sample: Compagnie Parento, Inc.).

## 1509: 4-HEPTEN-1-OL

*cis-4*-Heptenol.



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-CH_2OH$$

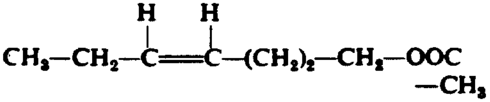
$C_7H_{14}O = 114.19$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Very powerful, fruity-green odor. In dilution mostly fruity and rather pleasant.

Developed in search of successful chemicals related to Hexenol, this unsaturated alcohol has never achieved the same popularity, again probably because the C-7-alcohols are so rare in Nature and the chemicals do not reproduce any distinctly natural odors.

## 1510: cis-4-HEPTENYL ACETATE



$CH_3{-}CH_2{-}\overset{H}{C}{=}\overset{H}{C}{-}(CH_2)_2{-}CH_2{-}OOC{-}CH_3$

$C_9H_{16}O_2 = 156.23$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

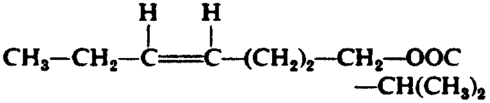
Very fresh, light, leafy-fruity odor with rosy undertones.

Suggested for use in perfume compositions, mainly as part of the topnote complex where fruity-green, refreshing effects are called for.

This ester has never achieved a success or popularity similar to that of the Hexenyl esters, all more natural in their odor types.

Prod.: by direct esterification of *cis-4*-Heptenol.

## 1511: cis-4-HEPTENYL-iso-BUTYRATE



$CH_3{-}CH_2{-}\overset{H}{C}{=}\overset{H}{C}{-}(CH_2)_2{-}CH_2{-}OOC{-}CH(CH_3)_2$

$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet, fatty-green, rather heavy odor. Under light, grassy notes there are fruity-floral, almost animal-heavy and quite tenacious nuances of nondescript character.

Again, the lack of similarity to any natural product seems to limit the possibilities for use of this ester. However, it is one of the most floral types of all the unsaturated (olefinic) esters.

Prod.: from *cis-4*-Heptenol by direct esterification with *iso*-Butyric acid under azeotropic conditions, or with *iso*-Butyric anhydride, using Phosphoric acid catalyst at slightly above room temperature.

## 1512: n-HEPTOXYACETIC ACID

$C_7H_{15}{-}O{-}CH_2COOH$

$C_9H_{18}O_3 = 174.24$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Somewhat fatty-oily odor, softer than that of Heptanol, and less fruity.

This acid has been suggested for use in perfume compositions, but the author finds that there is little, if any, use of the acid as such in perfumery. Certain esters may be used, but generally, the acid has only academic interest.

Prod.: from Sodium heptoxide and Monochloracetic acid, followed by saponification of the resulting ester.

31-157; see also: 66-788;

## 1513: HEPTYL ACETATE

"Acetate C-7".
*1*-Acetoheptane.
*n*-Heptyl acetate.
*n*-Heptanoic acetate.
Enanthic acetate.
Oenanthic acetate.

Note: The name "Oenanthic ether" for this ester is highly confusing, yet repeatedly used in flavor literature. See monograph: Ethyl oenanthate.

$CH_3(CH_2)_5CH_2{-}OOC{-}CH_3$

$C_9H_{18}O_2 = 158.24$

Colorless liquid. Sp.Gr. 0.87. B.P. 192° C.

Insoluble in water, miscible with alcohol and oils. Soluble in Propylene glycol.

Fruity, fatty-green and slightly floral odor with pleasant, leafy undertones. The delicate, leafy notes resemble those found in Applerose or Hiprose. Some observers find an earthy-green or mushroom-like note.

This acetate finds some use in perfume compositions, mainly as part of the topnote complex for Rose bases or other florals, also in green floral or foliage-green notes in non-floral bases. It lends a pleasant freshness even to Citrus compositions and blends equally well with Geranium oil, etc.

In flavor compositions, traces are used for imitation Banana, Berry, Melon, Pear, Pineapple, etc.

The normal concentration is as low as 3 to 5 ppm in the finished product.

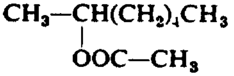
G.R.A.S. F.E.M.A. No.2547.

Prod.: by direct esterification of *n*-Heptanol with Acetic acid under azeotropic conditions, or with Acetic anhydride.

4-59; 26-568; 31-130; 35-61; 77-182; 86-57; 160-770; B-II-134; 140-135;

## 1514: secondary-HEPTYL ACETATE

Methyl amyl carbinyl acetate.
*2*-Heptanyl acetate.



$$\begin{array}{l} CH_3-\underset{|}{C}H(CH_2)_4CH_3 \\ \quad\;\, OOC-CH_3 \end{array}$$

$C_9H_{18}O_2 = 158.24$

Colorless liquid. Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Pleasant, warm, sweet, slightly fruity-balsamic odor with some resemblance to Opopanax and Myrrh.

Has been suggested for use in perfume compositions, mainly as a modifier in Chypre bases, Oriental fragrances, etc.

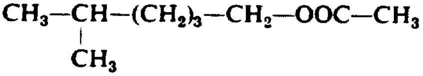
However, it does not seem to lend any very interesting note, and it does not have sufficient power to become a standard ingredient in competition with many chemicals of similar odor type.

Prod.: by Acetylation of Methyl amyl carbinol (*2*-Heptanol).

31-122;

## 1515: iso-HEPTYL ACETATE

*2*-Methyl hexyl acetate.



$$\begin{array}{l} CH_3-\underset{|}{C}H-(CH_2)_3-CH_2-OOC-CH_3 \\ \quad\;\, CH_3 \end{array}$$

$C_9H_{18}O_2 = 158.24$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

A rather uninteresting, fruity-green odor. Overall refreshing, but not very powerful, and not resembling any particular natural material.

In the author's opinion, there is little, if any, use of or interest for this material in perfumery.

Prod.: by Acetylation of *2*-Methylhexanol.

31-122; B-I-416;

## 1516: HEPTYL ACETOACETATE

Heptyl-*3*-oxobutanoate.

$C_7H_{15}-OOC-CH_2-CO-CH_3$

$C_{11}H_{20}O_3 = 200.28$

Colorless, oily liquid.

Insoluble in water, soluble in alcohol and oils.

Pleasant, oily-green, rich and sweet odor with vinous undertone and moderate tenacity.

This ester has found use in perfume compositions, mainly in specialties and bases intended for topnote work in the Citrus and light-floral type. The ester is rarely sold under its proper chemical name, but it enters a number of very useful bases of fresh, green-citrusy character and unusual power.

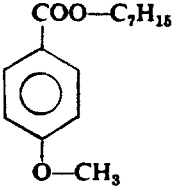
It performs very well with the equally clandestine Hydroxycaproic aldehydes and related aldehydes, acetals, etc. and it can be used with or without Citral – it gives a lemony effect if there are lemony materials present to be enhanced, while it has a similar lifting effect upon Bergamot and other Citrus oils. Light florals, such as Muguet and Freesia or the more imaginary waterlily type may also benefit from traces of the title aldehyde or compositions made thereof.

Prod.: from Heptanol and Diketen.

See also monograph: Ethyl-*beta*-ketopelargonate, an empirical isomer.

## 1517: n-HEPTYL ANISATE

Heptyl-*para*-methoxybenzoate.



$C_{15}H_{22}O_3 = 250.34$

Colorless oily liquid. Sp.Gr. 1.02.
B.P. 276° C.

Insoluble in water, soluble in alcohol and oils. Practically insoluble in Propylene glycol.

Faint, but sweet, fruity-winey odor, occasionally with an Almond-like undertone.

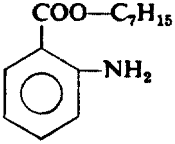
Although this ester has been suggested for use in perfumes, it is the author's impression, that this material rarely, if ever, is used in perfumes. Its effect in fragrances is not unusual, and it is overall weak and uncharacteristic.

Prod.: by direct esterification of *n*-Heptanol with Anisic acid under azeotropic conditions.

4-59; 34-681;

## 1518: n-HEPTYL ANTHRANILATE

Heptyl-*ortho*-aminobenzoate.



$C_{14}H_{21}NO_2 = 235.33$

Colorless or pale straw-colored viscous liquid.
B.P. 320° C. Sp.Gr. 1.02.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

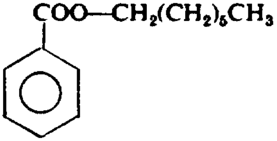
Sweet, woody-floral, somewhat green, but very weak odor, remotely reminiscent of Petitgrain.

In the author's opinion, this ester is too weak and too deficient in characteristic notes to become a standard perfumery item.

Prod.: from Isatoic anhydride and *n*-Heptanol. Also produced from Anthranilic acid and Heptanol, or from Methyl anthranilate and Heptanol.

35-59;

## 1519: n-HEPTYL BENZOATE



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid. B.P. 257° C.
Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Mild woody-green almost weedy or Sage-like odor of good tenacity. The odor type is, however, rather unnatural, not exactly pleasant (like damp wood) and often further spoiled by trace impurities of metallic odor, etc.

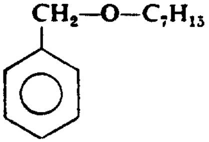
This ester has been recommended for use in non-floral perfume compositions such as Chypre and Fougère, but it does not seem to contribute much to fragrances at all.

Prod.: by direct esterification of *n*-Heptanol with Benzoic acid under azeotropic conditions.

4-59; 35-61; 86-57;

## 1520: HEPTYL BENZYL ETHER

Benzyl heptyl ether.
"Benzyl heptyl oxide".



$C_{14}H_{22}O = 206.33$

Colorless liquid. B.P. 265° C. Sp.Gr. 0.90.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar "metallic" odor, yet remotely reminiscent of the odor of Geranium leaves. Some descriptions include the word "Bitter Almond" but the author of this work believes that such odor must derive from impurities and not from good grade Benzyl heptyl ether. Dibenzyl, which has a "Bitter-Almond"-like odor, is formed as a by-product if the ether is made as indicated below.

Finds a little use in Oriental or Balsamic fragrance types, also as a fixative-blender. Like most ethers, it is very stable in soap.

Prod. from Benzyl alcohol and *n*-Heptanol. If the condensation is undertaken by way of Sulfuric acid addition, some Dibenzyl will form as a by-product. See above.

4-22; 86-23;

## 1521: n-HEPTYL-n-BUTYRATE

*n*-Heptyl-*n*-butanoate.

$CH_3(CH_2)_5CH_2—OOC—C_3H_7$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Sp.Gr. 0.88. B.P. 225° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet-green, yet fresh and slightly Tea-like odor. In higher concentration also reminiscent of Violet leaf.

The subject ester could find use in perfume compositions, but it is rarely mentioned as a perfume material. It introduces interesting nuances in fruity-green topnote complexes for Chypre or Aldehyde-types, and it can be used as a modifier in "Cucumber" odor, sometimes called for in certain cosmetic preparations. It blends excellently with Clary Sage and with the new American Mentha citrata oils (Todd # 664 in particular).

In flavor compositions, this ester adds freshness and fruity-green aroma to imitation Raspberry, Apricot, Melon, Plum, and in floral and Violet type flavors.

The concentration used is normally very low, about 0.5 to 3 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2549.

Prod.: by direct esterification of *n*-Heptanol with *n*-Butyric acid under azeotropic conditions.

4-59; 33-732; 35-61; 86-57;

## 1522: HEPTYL-iso-BUTYRATE

*n*-Heptyl-*iso*-butanoate.
*n*-Heptyl-2-methylpropanoate.
*n*-Heptyl dimethylacetate.

$CH_3(CH_2)_5CH_2—OOC—CH(CH_3)_2$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. B.P. 212° C. Sp.Gr. 0.86.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Peculiar, complex fruity odor with distinctly herbaceous, sweet undertones. There are notes resembling Chamomile and other notes resembling Apple, and there is an overall green floral odor.

The taste is sweet, herbaceous-fruity, slightly warm and with a floral nuance.

This ester finds some use in perfumery for variation effects in Rose and Violet, and as a modifier for the Chamomile topnote theme. It blends very well in Violet and Cyclamen notes.

Traces of the ester are used in flavor compositions for imitation Apricot, Coconut, Orange, Peach, Pineapple, Plum, etc.

Concentrations are as low as 0.5 to 3 ppm in the finished product.

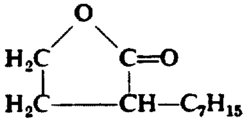
Prod.: by direct esterification of *n*-Heptanol with *iso*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2550.

4-59; 31-130; 35-61; 140-139;

## 1523: alpha-HEPTYL-gamma-BUTYROLACTONE

*alpha*-Undecanolide-*1,4*.
*alpha-n*-Undecyllactone.
An isomer of the so-called "Peach Aldehyde".
(See also: *gamma*-Undecalactone).



$C_{11}H_{20}O_2 = 184.28$

Pale straw-colored or almost colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Sweet fruity, Peach-like and musky odor, yet overall fresher, not as heavy as the *gamma*-isomer. Very good tenacity.

Sweet and fruity taste, yet somewhat more animal than that of the *gamma*-isomer.

Although overall very pleasant and interesting, this material has not achieved wide acceptance, perhaps because of its considerably higher price.

It could undoubtedly find use in perfumes and flavors as a modifier for the conventional "Peach Aldehyde".

Prod.: (several methods) e. g. from Heptyl malonic ester and Ethylene oxide.

31-170; 156-229; 159-418;
See also: *gamma*-Undecalactone.
*delta*-Undecalactone.

## 1524: n-HEPTYL CAPRATE

Heptyl caprinate.
Heptyl decanoate.
Heptyl decylate.

$C_7H_{15}—OOC—C_9H_{19}$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid. B.P. 290° C.
Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Mild winey-brandy-like odor reminiscent of the odor of "tail fractions from rectification of Fusel oil", yet much milder. Remotely reminiscent of Cognac oil.

Suggested for use in perfume compositions. Traces of this ester may add a certain "mellowness" to perfumes of herbaceous type, and it can occasionally be used for floral notes to add the desirable oily-winey-creamy note as for instance displayed in good Ylang Extra.

The ester is, to the author's knowledge, not used in flavor compositions, although it might well contribute interesting aroma to Rum and Brandy flavor imitations.

Prod.: by direct esterification of *n*-Heptanol with Decanoic acid (Capric acid) under azeotropic conditions.

4-59; 35-61;

## 1525: n-HEPTYL CAPROATE

*n*-Heptyl-*n*-hexanoate.
Heptyl hexylate.

$C_7H_{15}$—OOC—$C_5H_{11}$

$C_{13}H_{26}O_2 = 214.35$

Colorless liquid. B.P. 260° C. Sp.Gr. 0.87.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Fresh-green, foliage and vegetable-like odor, reminiscent of the odor of freshly crushed leaves and stems, or the juice from same. Remotely reminiscent of Violet leaf greenness.

The subject ester finds a little use in perfumery as a modifier for the conventional materials of "green" notes. Heptyl caproate supplies a softer, more "juicy" greenness than most of the other materials, and it is quite versatile. It introduces very pleasant freshness in a Fougère, and has the ability of taking the dullness out of Amyl salicylate or other heavy chemical odors.

The ester could find use in flavor compositions, but it is not specifically listed as G.R.A.S. in the American Federal Register, and can not be used in the United States as a food flavoring.

It is most conceivably used in other countries. There are no reports indicating that Heptyl caproate is particularly toxic as compared to its homologues.

Prod.: by direct esterification of *n*-Heptanol with Caproic acid under azeotropic conditions.

4-59; 31-130; 34-1230; 35-61; 86-57;

## 1526: n-HEPTYL CAPRYLATE

Heptyl octanoate.
Heptyl octylate.

$C_7H_{15}$—OOC—$C_7H_{15}$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 290° C.

Insoluble in water, soluble in alcohol and oils.

The odor of this ester does not remind of any particular natural material, and it is therefore a rather uninteresting ester. There are oily-fruity notes of the type often found as undesirable topnotes in certain essential oils (Amyris, Cedarwood, etc.), notes which are sometimes described as "odor of green potatoes or of Peanuts".

Yet, the ester does contribute interesting notes to fruit flavors, often exactly the missing "oily-fruity" undertone, hard to find in the conventional esters.

Traces are used in various fruit complexes, and the concentration of about 1 ppm in the finished product is quite normal.

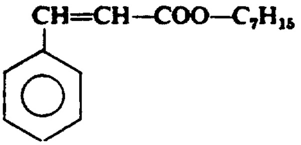
G.R.A.S. F.E.M.A. No.2553.

Prod.: by direct esterification of *n*-Heptanol with *n*-Octanoic acid (Caprylic acid) under azeotropic conditions.

NOTE: Heptyl esters are extremely rare in Nature, and it is most conceivable that one does not immediately appreciate the odor of many such esters.

35-61; 86-57;

## 1527: n-HEPTYL CINNAMATE



$C_{16}H_{22}O_2 = 246.35$

Colorless or pale straw-colored, viscous liquid.

This ester tends to polymerize upon storage. It shows increasing viscosity and turbidity, and decreasing odor and solubility.

Insoluble in water, soluble in alcohol and oils, practically insoluble in Propylene glycol.

Mild, floral-green, somewhat bark-like odor with a woody-earthy undertone, remotely reminiscent of Hyacinth.

The tendency of this material to polymerize is often the main reason for the perfumers not to use it. Unfrequently used materials show too much odor variation and such display of instability is enough to kill a perfume material. The ester could find some use in Hyacinth and Lilac bases as a fixative and modifier. Once incorporated in a perfume oil, it shows less tendency to polymerize, presumably due to the dilution of the material.

The ester finds a little use in flavor compositions. Again, it is interesting to note that the effects for which it is used, are actually effects deriving from decomposition: Cherry, Bitter-almond-Apricot, etc. all depend upon the Benzaldehyde-like note emanating from the ester when it is decomposing. A virtually pure ester does not have such odor or flavor characteristics.

Traces of the ester are also used in various Berry and Grape flavor types. The normal concentration is about 1 to 6 ppm, but since the ester is used as a fixative in chewing gum, its concentration in that product may reach 250 to 280 ppm.

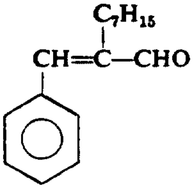
G.R.A.S. F.E.M.A. No.2551.

Prod.: by direct esterification of *n*-Heptanol with Cinnamic acid under azeotropic conditions.

4-59; 34-462; 35-59; 86-57;

## 1528: alpha-n-HEPTYL CINNAMIC ALDEHYDE

Heptyl cinnamal.



$C_{16}H_{22}O = 230.35$

Pale yellowish, oily liquid. B.P. 288° C. Sp.Gr. 0.94.

Insoluble in water, soluble in alcohol and oils. Insoluble in Propylene glycol.

Very faint, mild, sweet-oily odor. In compositions with more volatile ingredients, this aldehyde shows a floral effect.

Although actually just a member of a long line of research chemicals developed in search of good variations of Amylcinnamic aldehyde, this aldehyde has occasionally found use in perfumery. However, it has not become a shelf-item such as its lower homologue, Hexylcinnamic aldehyde.

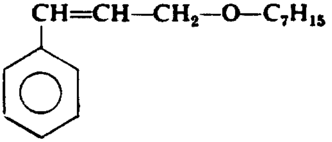
There is perhaps a slightly greener note to the floral-oily effect of this aldehyde, but overall it is too weak and not sufficiently distinctive to be used widely as a Jasmin floralizer in various floral compositions.

Prod.: by condensation of Benzaldehyde with *n*-Nonanal (Claisen condensation).

31-51; 93-150;

## 1529: HEPTYL CINNAMYL ETHER

Cinnamyl heptylether.



$C_{16}H_{24}O = 232.37$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet and tenacious, warm-woody, somewhat balsamic odor. Not reminiscent of any particular natural material.

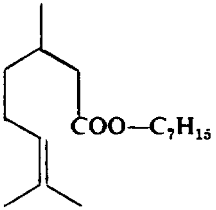
Has been suggested for use in perfume compositions, but is very rarely offered commercially.

It may find a little use as a fixative and modifier in Oriental fragrance types of heavy-balsamic florals.

Prod.: From Cinnamic alcohol and *n*-Heptanol by dehydration.

31-144;

## 1530: HEPTYL CITRONELLATE



$C_{17}H_{32}O_2 = 268.44$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 278° C.

Insoluble in water, soluble in alcohol and oils.

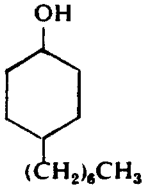
Peculiar metallic-medicinal odor, not very pleasant or natural.

Probably developed in an attempt to find "green" esters of Citronellic acid, this ester does not seem to offer any interesting notes and the author believes that it can be considered of academic interest only.

4-59;
see also: Chemical Abstracts, 43, 4633 (1949).

## 1531: para-HEPTYL CYCLOHEXANOL

*1*-Oxy-*4*-heptyl cyclohexane.



$C_{13}H_{26}O = 198.35$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Camphoraceous-green, somewhat woody and quite tenacious odor. Not reminiscent of any particular natural material.

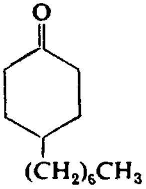
Has been suggested for use in perfume compositions. It is the author's impression there is very little, if any, use of this alcohol at all in perfumery.

Prod.: by. hydrogenation of *para*-Heptylphenol.

31-25; 86-57;
U.S. pat. 2.100.468 (1937) (E. I. duPont de Nemours) suggests that this material is used in perfumes.

## **1532:** para-**HEPTYL CYCLOHEXANONE**

*1*-Oxo-*4*-heptylcyclohexane.



$C_{13}H_{24}O = 196.34$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

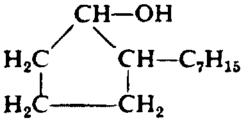
Powerful, camphoraceous-woody, somewhat green and Orris-like odor of considerable tenacity.

Suggested for use in perfumes, this ketone does not have the versatility of the more well-known members of the alkyl-substituted Cyclohexanones. It is not quite as powerful and does not blend satisfactorily with the Ionones, an ability well appreciated in certain lower homologues. This ketone could find some use in soap perfumes where its power and stability come in handy, but again, its odor is generally considered inferior to that of the Amyl- and Butyl- homologues.

Prod.: by oxidation of *para*-Heptyl cyclohexanol.

## **1533:** 2-n-**HEPTYL CYCLOPENTANOL**

"Tetrahydrojasmone" (somewhat misleading name).



$C_{12}H_{24}O = 184.32$

Colorless or pale straw-colored oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Slightly soluble in Propylene glycol.

Powerful and diffusive, fruity-floral and very sweet odor of moderate tenacity. It is less floral and more fruity than the corresponding ketone (Heptyl cyclopentanone, a well-known specialty) and it has a similar, but sweeter greenness. Overall, however, it does not have the power of the ketone.

This alcohol has been suggested for use in perfume compositions as a Jasmin-type material and a modifier for the many available ketones related to Jasmone.

In the author's opinion, it has its own field of application and does not compete with the ketones as far as Jasmin-effect is concerned. The subject alcohol could find good use as a topnote ingredient in many aldehydic, aldehydic-green and fruity-green fragrance complexes, and in more fresh types of floral fragrance. A special use would be in Lavender compositions.

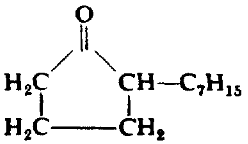
The fact that this material is comparatively rare in the perfume chemicals lists could indicate that there is not much interest in it.

Prod.: by catalytic reduction of Heptyl cyclopentanone.

86-127;

## **1534:** 2-n-**HEPTYL CYCLOPENTANONE**

"Alismone" (Givaudan).
"Fleuramone" (I.F. & F.).
*alpha*-Heptyl cyclopentanone.



$C_{12}H_{22}O = 182.31$

Almost colorless or very pale straw-colored oily liquid. Sp.Gr. 0.89.

Practically insoluble in water, soluble in alcohol and oils.

Floral-green, fruity and warm, somewhat herbaceous odor with overall resemblance to certain notes in Jasmin. One manufacturer also describes the odor as "Rue-like" (The Rue-odor is partly due to a C-11 alifatic ketone, Methyl nonyl ketone).

Powerful, fruity-floral and green-winey-herbaceous, but somewhat bitter taste.

This ketone is used in perfume compositions for Jasmin, Honeysuckle, Reseda, Chypre, and many other fruity floral types.

It blends exceptionally well with macrocyclic musks and Undecanolide and related materials. It also lends freshness and power to Lavender and other non-floral fragrance types.

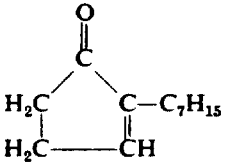
The author doubts that this ketone could be used in flavors, since it has a bitter taste unless very highly diluted.

Prod.: by catalytic reduction of Heptylidene cyclopentanone (which is part of the commercial product known as "*iso*-Jasmone") French pat. 779789 (Givaudan 1935).

34-1211; 106-44;

## 1535: HEPTYL CYCLOPENTENONE

"Homo-*iso*-jasmone".
*2*-Heptylcyclopenten-*2*-one-*1*.



$C_{12}H_{20}O = 180.29$

Pale yellowish or straw-colored oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful floral-fruity odor, overall less fruity and more floral than the average commercial type of "*iso*-Jasmone". Moderate tenacity, and a somewhat green topnote seems to accompany the odor for most of the duration, except for the extreme dryout notes which are more floral.

Bitter floral taste in concentrations down to a few ppm.

It has been stated repeatedly that the odor of this ketone is superior to that of "*iso*-Jasmone", but the author finds that there are so-called "*iso*-Jasmones" in the trade of definitely superior odor performance.

In any event, it should be encouraging to have a well-defined chemical with the odor qualities of a good *iso*-Jasmone and in the same price category. For such materials there are countless uses in perfumery: not only in Jasmin bases and perfumes, but virtually in all floral and many herbaceous or non-floral types as well. In combination with Undecanolide or other lasting fruity notes, it may produce new and interesting topnotes, or it can be twisted towards a greener, even a Citrus-like note with the proper additives.

Prod.: by cyclization of Dodecenoic acid.

156-223;

## 1536: HEPTYL DECYL ETHER

Decyl heptyl ether.
Heptyl decyl oxide.

$C_7H_{15}\text{—}O\text{—}C_{10}H_{21}$

$C_{17}H_{36}O = 256.48$

Colorless oily liquid. B.P. 280° C.
Sp.Gr. 0.82.

Insoluble in water, soluble in alcohol and oils.

Rather nondescript, herbal odor. Green-oily, almost fresh, but not reminiscent of any particular natural material.

The development of various chemical families for use in perfumery seems to come in waves. Once the Heptyl ethers were in the limelight, and a great number of Heptylesters and ethers were manufactured. Only a few of them had odors of true interest to the perfumer. Many had "metallic" notes, and the common odor is a variation of the "green" note. The ethers are, in general, very stable in soap, and many are quite powerful odorants.

The author believes that this ether is of very little interest to the creative perfumer.

Prod.: from *n*-Heptanol and *n*-Decanol by dehydration.

4-41; 37-176;

## 1537: HEPTYL DODECYL ETHER

Dodecyl heptyl ether.
Lauryl heptyl ether.
Lauryl heptyl oxide.

$C_7H_{15}—O—C_{12}H_{25}$

$C_{19}H_{40}O = 284.53$

Colorless oily liquid. B.P. 277° C. Sp.Gr. 0.82.

Insoluble in water, soluble in alcohol and oils.

Very faint, fatty-oily "laundry"-like odor. The odor is somewhat reminiscent of the odor of fresh vegetable oils.

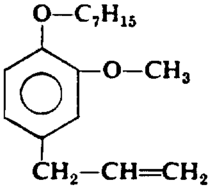
Although this ether has been mentioned in literature as a perfume chemical, the author doubts that it can be classified as such. It has very little to offer, and no unusual effects.

Prod.: from *n*-Heptanol and Lauryl alcohol by dehydration.

4-80;

## 1538: HEPTYL EUGENOL

Eugenol heptylether.
*3*-Methoxy-*4*-heptoxy allylbenzene.



$C_{17}H_{26}O_2 = 262.40$

Colorless or pale straw-colored oily liquid. B.P. 270° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils, practically insoluble in Propylene glycol.

Leather-like, somewhat tarry and dry odor (topnote), becoming sweeter on longer study, more fruity on dryout. Overall a "Cuir de Russie" type with sweet undertones.

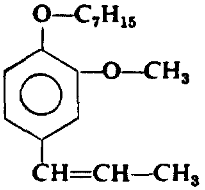
This ester has been suggested for use in perfume compositions as part of the "leather"-complex for so-called "Cuir de Russie" fragrance types, and for various types of "Men's fragrances" of the recently revived kind. It blends well with Ionones, Ylang or Cananga oils, Amylsalicylate, Hydroquinone dimethylether, Oakmoss products, etc.

Prod.: from *n*-Heptyl bromide and Eugenol in alcoholic alkaline solution.

34-1116; 28-629; 86-51;

## 1539: HEPTYL-iso-EUGENOL

*iso*-Eugenol heptylether.
*3*-Methoxy-*4*-heptoxy propenyl benzene.



$C_{17}H_{26}O_2 = 262.40$

Pale yellowish or straw-colored viscous liquid.
B.P. 276° C. Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils. Insoluble in Propylene glycol.

Mild and very sweet, also fruity and very tenacious odor, remotely reminiscent of over-ripe fruit (Apples). Contrary to the Heptyl eugenol this ether is not tarry, not leather-like.

Suggested for use in perfume compositions. Very rarely offered from the regular producers of Aroma chemicals, this ether is not likely to be present on many shelves in perfumers' laboratories, and it does not offer very outstanding effects or give irreplaceable notes.

Prod.: by Isomerization of Heptyl eugenol, or from *iso*-Eugenol in alcoholic alkali solution with Heptyl bromide.

4-72; 34-1116;

## 1540: HEPTYL FORMATE

*n*-Heptyl methanoate.

$C_7H_{15}—OOCH$

$C_8H_{16}O_2 = 144.22$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 178° C.

Insoluble in water, soluble in alcohol, Propylene glycol and oils.

Somewhat sharp, fruity-fatty, Apple and Plum-like, remotely Orris-like odor of moderate tenacity.

Sweet, rather heavy-fruity taste, reminiscent of Apple and Plum.

Apart from a possible use as part of topnote complexes in perfumes of woody-fruity character, there is probably very little application of this ester in fragrances. It gives interesting effects in support of Elderflower absolute ("Tombacco", etc.).

Heptyl formate is used sparingly in flavor compositions for imitation Apricot, Peach, Plum, Raspberry, Blackcurrant, Gooseberry, Rum, etc.

The concentration used is equivalent to about 1 to 4 ppm in the finished product.

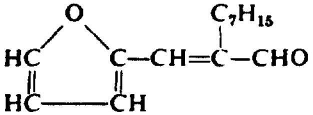
G.R.A.S. F.E.M.A. No.2552.

Prod.: by direct esterification of *n*-Heptanol with Formic acid in presence of a catalyst.

4-59; 26-568; 31-130; 35-59; 35-61; 77-171; 160-1000; B-II-22; 140-132;

## 1541: alpha-HEPTYL FURFURACROLEIN

*alpha-n*-Heptyl-*beta-2*-furylacrolein (correct name).
*alpha*-Furfurylidene nonanal.



$C_{14}H_{20}O_2 = 220.31$

Pale yellow or yellow oily liquid.

Insoluble in water, soluble in alcohol and oils.

Very mild green-herbaceous and warm odor of considerable tenacity.

This aldehyde was developed as member of a long series of alkylsubstituted Furfurals in search of interesting relatives to Amylcinnamic aldehyde (analogous from Benzaldehyde).

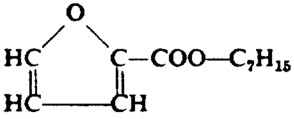
Although this aldehyde does display interesting notes, it has not become a standard item yet, and probably never will. After 45 years of existence and increasing popularity, Amylcinnamic aldehyde is very difficult to substitute.

Prod.: by Claisen type condensation of Furfural and Nonyl aldehyde.

31-40; 93-150;

## 1542: n-HEPTYL FUROATE

Furan-*alpha*-carboxylic acid, *n*-Heptylester.
*n*-Heptyl pyromucate.



$C_{12}H_{18}O_3 = 210.28$

Colorless liquid. Sp.Gr. 1.00. B.P. 280° C. (decomposes).

Insoluble in water, soluble in alcohol and oils.

Warm, somewhat caramellic-herbaceous odor of good tenacity. A complex of green-herbal and very sweet, deep notes produces an almost floral character.

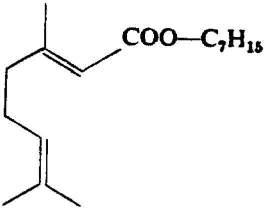
Although this ester displays a very unusual odor picture, it does not seem to have achieved much popularity among perfumers or flavorists.

It could undoubtedly find use not only in the reconstruction of essential oils, but also as a modifier in modernized Lavender fragrances, in Jasmin variations, and in new odors for room fresheners, etc.

Prod.: by direct esterification under azeotropic conditions.

4-24; 160-1008;

## 1543: HEPTYL GERANIATE



$C_{17}H_{30}O_2 = 266.43$

Colorless or pale straw-colored viscous liquid. B.P. 287° C. Sp.Gr. 0.90.

Insoluble in water, soluble in alcohol and oils.

Peculiar sweet-coumarinic, slightly woody-floral odor resembling Cassie, Mimosa and New Mown Hay, yet milder than the latter. Excellent tenacity.

This rare ester has been suggested for use in floral fragrances Oriental bases, woody complexes, etc. It blends well with Oakmoss, Patchouli, Rose, and with the herbaceous odors.

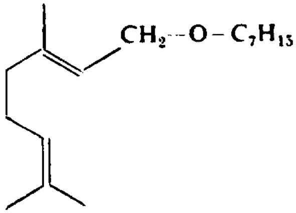
Only occasionally offered commercially there is not much chance that it will become an everyday item, and it does not contribute such very unusual effects that it would be further promoted by the manufacturers of perfume chemicals.

Prod.: (several methods), e. g. from Geranic acid and *n*-Heptanol.

4-59; 31-130;

## 1544: HEPTYL GERANYL ETHER

Geranyl heptyl ether.
Heptyl geranyl oxide.



$C_{17}H_{32}O = 252.44$

Colorless liquid. Sp.Gr. 0.84. B.P. 262° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-green, citrusy odor with some resemblance to notes in Lime oil. Good tenacity.

With a comparatively unusual odor, this ether should have some chances of becoming a regularly used perfume chemical. It is stable under normally alkaline conditions and against the most common chemical exposures in soaps and cosmetics. With the Lime theme so extremely popular lately, it could possibly find use in new variations of that odor type.

Prod.: (several methods), e. g.: from Geranyl chloride plus Sodium heptoxide in Heptyl-alcohol.

4-56; 31-144;

## 1545: n-HEPTYL HEPTOATE

*n*-Heptyl-*n*-heptanoate.
Heptyl heptylate.
"Oenanthic ether" (old, misleading name)*).

$C_7H_{15}$—OOC—$C_6H_{13}$

$C_{14}H_{28}O_2 = 228.38$

Colorless liquid. Sp.Gr. 0.86. B.P. 274° C.

Insoluble in water, soluble in alcohol and oils.

Winey-green, rather fatty, fermentation odor of considerable tenacity. The green undertones are much less grassy than those of the Hexylesters, and not as natural, more fatty.

This ester finds a little use in perfumery, mainly in Fougeres and Chypres, where it may blend with Amylsalicylate, Coumarin, herbaceous oils and Citrus oils. It is not a very popular chemical, maybe because it does not reproduce any distinctly natural note.

In flavors, it finds a limited use as a modifier in imitation Cognac, and in traces in certain vegetable flavor types. It has a special mission in some Bitter Almond flavors, where it can introduce a fresh and pleasant topnote to the otherwise sickly sweet Benzaldehyde-type flavor.

Prod.: by direct esterification of *n*-Heptanol with Heptanoic acid under azeotropic conditions.

4-59; 7-205; 26-568; 35-61; 86-57; 103-189; 160-968; B-II-340;

*) see also: Heptyl acetate.
Ethyl heptoate.
Ethyl oenanthate.

## 1546: HEPTYLIDENE ACETONE

Oenanthylidene acetone.
*3*-Decen-*2*-one.

$CH_3(CH_2)_5CH{=}CH-CO-CH_3$

$C_{10}H_{18}O = 154.25$

Almost colorless mobile liquid.

Practically insoluble in water, soluble in alcohol and oils.

Fruity-floral, somewhat Jasmin-like, fatty-green and waxy odor with some resemblance to Orris undertones.

This ketone has found a little use in perfume compositions as component of certain types of Jasmin bases. It may also find some use in other florals, since it blends well with the Ionones and with woody as well as certain Citrus complexes. It is quite powerful and relatively stable towards alkali and other chemical reactants commonly encountered in cosmetic preparations.

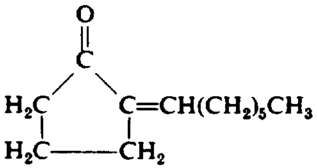
Approved for food flavor use by the American F.R.

Prod.: by condensation of Heptaldehyde and Acetone.

4-59; 7-205; 7-306; 31-84; 86-57;

## 1547: 2-n-HEPTYLIDENE CYCLOPENTANONE

*alpha*-Heptylidene cyclopentanone.



$C_{12}H_{20}O = 180.29$

Pale yellowish or almost colorless oily liquid. B.P. 242° C.

Insoluble in water, soluble in alcohol and oils.

Powerful floral, slightly oily-fruity odor of good tenacity. Less fruity than the so-called "*iso*-Jasmone", but somewhat sharper than the better-known Heptyl cyclopentanone. Overall character of a floral-fruity Jasmin type chemical.

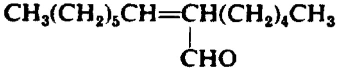
This ketone has been suggested for use as a Jasmin component in perfume compositions, but it has not achieved the same popularity as the above mentioned related ketones. It could be on account of the sharper topnote of the subject ketone, an effect which seems to limit the use of this material.

Prod.: by condensation of Cyclopentanone and Heptaldehyde.

31-85; 31-86; 34-1211;

## 1548: HEPTYLIDENE HEPTANAL

"Di-heptenal".
*2*-Amyl nonetal.



$$CH_3(CH_2)_5CH{=}\underset{\displaystyle CHO}{\underset{|}{C}}H(CH_2)_4CH_3$$

$C_{14}H_{27}O = 211.37$

Yellowish oily liquid. B.P. approximately 285° C.

Insoluble in water, soluble in alcohol and oils.

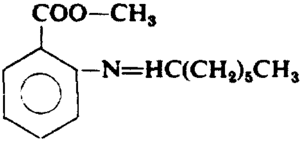
Fatty and very "oily", slightly green, but overall "rancid" type of odor.

Occasionally used in masking odors for industrial purposes.

Prod.: by condensation of 2 Mol. Heptaldehyde as a side reaction in the manufacturing of Amylcinnamic aldehyde. It is present in the reaction mixture and in the crude distillate of ACA because its boiling point is very close to that of the ACA. Heptylidene heptanal is therefore a comparatively large component of the "tail" fractions of ACA, a by-product often used in industrial masking odors.

## 1549: HEPTYLIDENE METHYLANTHRANILATE

Oenanthylidene Methylanthranilate.
Heptaldehyde-Methylanthranilate, Schiff's base.
"Heptylique".
Methyl-*N*-heptylidene anthranilate.



$C_{15}H_{21}NO_2 = 247.34$

Intensely yellow, viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very sweet, green-floral, herbaceous-Orangeblossom-type odor of good tenacity. It is a common feature of Schiff's bases, that their odor is strongly dependent upon the method of preparation and the ratio used of the two components in the reaction. In this particular case, any small surplus of the aldehyde is particularly noticeable in the odor of the base.

Suggested for use in various heavy florals, including Jasmin, Narcisse, Jonquil, etc.

Prod.: by simple condensation of Heptaldehyde with Methylanthranilate and removal of the water formed.

## 1550: HEPTYL LAURATE

Heptyl dodecanoate.
*n*-Heptyl dodecylate.

$C_7H_{15}—OOC—C_{11}H_{23}$

$C_{19}H_{38}O_2 = 298.51$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Fatty-waxy, weak and somewhat Stearin-like odor of considerable tenacity.

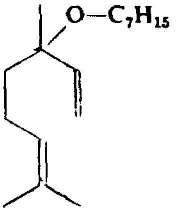
This ester has found very little use in perfume compositions. Occasionally it finds its way into certain floral bases, such as Tuberose or Lily, where it may supply fairly natural waxy "petal-like" notes accompanied by a discrete greenness.

Prod.: by direct esterification of *n*-Heptanol with Dodecanoic acid under azeotropic conditions.

4-59; 35-59;

## 1551: HEPTYL LINALYL ETHER

Linalyl heptyl ether.



$C_{17}H_{32}O = 252.44$

Colorless liquid. B.P. 227° C. Sp.Gr. 0.84.

Insoluble in water, soluble in alcohol and oils.

Earthy-green, herbaceous and comparatively powerful odor of moderate tenacity.

This ester comes out of a great number of homologues from a research program aiming at the development of new and interesting Linalyl ethers. It appears, however, that hardly any of the ethers have achieved a popularity worth mention, while several of the higher homologues of Linalool have become standard perfumery chemicals in common use.

The author believes that the subject ether, and many others, will quickly become obsolete in perfumery.

4-83; 31-144;

## 1552: HEPTYL MYRISTATE

Heptyl tetradecanoate.

$C_7H_{15}$—OOC—$C_{13}H_{27}$

$C_{21}H_{42}O_2 = 326.57$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 310° C.

Insoluble in water, soluble in oils and alcohol.

Very weak, waxy, mild odor, characteristic of Stearic-Palmitic compounds. Excellent tenacity, and in pure esters, a pleasant overall odor, while poorer grades may show "rancid" type fatty notes, definitely disagreeable and useless.

The ester could find a little use in perfume compositions for floral bases, e. g. Tuberose, Jonquil, Lily etc. where the waxy character may duplicate the natural "petal" odor.

Prod.: by direct esterification of *n*-Heptanol with Myristic acid under azeotropic conditions.

4-60; 35-59; 86-57;

## 1553: n-HEPTYL NONYLATE

Heptyl pelargonate.
Heptyl nonanoate.

$C_7H_{15}$—OOC—$C_8H_{17}$

$C_{16}H_{32}O_2 = 256.43$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 273° C.

Insoluble in water, soluble in alcohol and oils.

Mild, winey-sweet, oily and floral odor with Orange/Orangeblossom and Rose-like undertones.

This ester finds a little use in perfumery mainly in light floral perfumes, and occasionally in Oriental fragrances as a companion to Opopanax-notes with which the ester blends excellently.

It may also provide interesting topnotes in combination with Angelica seed oil or Cognac oil in herbaceous fragrance types.

The ester is occasionally used in flavor compositions (not in the U.S.A., not listed as G.R.A.S.) particularly in imitation Cognac flavors.

Prod.: by direct esterification of *n*-Heptanol with Nonanoic acid under azeotropic conditions.

4-60; 35-61; 86-57; 140-143;

## 1554: HEPTYL NONYL ETHER

Nonyl heptyl ether.
Heptyl nonyl oxide.

$C_7H_{15}$—O—$C_9H_{19}$

$C_{16}H_{34}O = 242.45$

Colorless oily liquid. B.P. 264° C.
Sp.Gr. 0.82.

Insoluble in water, soluble in alcohol and oils.

Rather unpleasant fatty-oily odor, often described as reminiscent of the odor of "wet sheep" ("Lamb's wool odor").

This type of odor is rarely, if ever, called for in perfumery, and in the author's opinion, there is only academic interest in this ether.

Prod.: from *n*-Heptanol and *n*-Nonanol by dehydration.

4-105; 35-60; 37-176;

## 1555: HEPTYL OCTYL ETHER

Octyl heptyl ether.
Heptyl octyl oxide.

$C_7H_{15}—O—C_8H_{17}$

$C_{15}H_{32}O = 228.42$

Almost colorless oily liquid.
Sp.Gr. 0.82. B.P. 272° C.

Mild, sweet-oily odor with a peculiar earthy-green note, resembling the odor of freshly crushed (fresh) peanuts. Also resembling the odor of the green peel of potatoes or raw coffee beans.

Apart from a few very rare, possible applications in perfumery, there is probably not much use for this ether. Its peculiar odor resembles notes in Amyris oil, Vetiver oil and Cedarwood oil, when these oils are either too "fresh" or produced from "green" plant material. In all cases, an undesirable odor.

Prod.: from *n*-Heptanol and *n*-Octanol by dehydration.

31-176;

## 1556: n-HEPTYL OLEATE

Heptyl-9-octadecenoate.

$C_7H_{15}—OOC—C_{17}H_{33}$

$C_{25}H_{48}O_2 = 380.66$

Pale yellowish or almost colorless liquid. Sp.Gr. 0.87. B.P. 320° C.

Insoluble in water, soluble in alcohol and oils.

Very mild, oily-sweet odor, reminiscent of refined Peanut oil or good grade Olive oil.

Suggested for use in the reconstruction of certain flower absolutes, but otherwise probably not used in perfumes or flavors.

Prod.: by esterification of *n*-Heptanol with Oleic acid under azeotropic conditions.

35-59;

## 1557: n-HEPTYL PALMITATE

Heptyl hexadecanoate.

$C_7H_{15}—OOC—C_{15}H_{31}$

$C_{23}H_{46}O_2 = 354.62$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 315° C.

Insoluble in water, soluble in alcohol and oils.

Very mild oily odor, reminiscent of freshly refined Cod liver oil (no fishy notes!) or good grade Linseed oil.

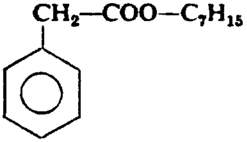
The ester could possibly find some use in the reconstruction of certain flower absolutes, but overall it appears to have only academic interest.

Prod.: from *n*-Heptanol by esterification with Palmitic acid under azeotropic conditions.

35-59;

## 1558: HEPTYL PHENYLACETATE

*n*-Heptyl-*alpha*-toluate.



$C_{15}H_{22}O_2 = 234.34$

Colorless, somewhat viscous liquid.
B.P. 265° C. Sp.Gr. 1.02.

Insoluble in water, soluble in alcohol and oils.

Green and sweet, yet fresh-earthy saplike or barklike odor with a trace of resemblance to Verbena (the non-lemony portion of Verbena odor).

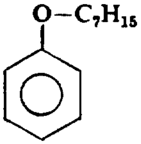
This ester has been suggested for use in perfume compositions, but its odor type is rather strange, and its effects not sufficiently unusual, beautiful or powerful to warrant any further promotion of this material.

Prod.: by esterification of *n*-Heptanol with Phenylacetic acid under azeotropic conditions.

34-246; 35-61;

## 1559: HEPTYL PHENYL ETHER

Phenyl heptyl ether.
*n*-Heptoxybenzene.
Heptyl phenyl oxide.



$C_{13}H_{20}O = 192.30$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Green-balsamic, warm-herbaceous odor, remotely reminiscent of Myrrh and Opopanax, but much inferior with respect to tenacity.

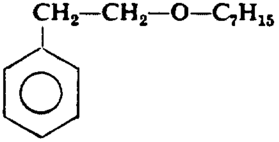
Very rarely offered commercially, this ether finds perhaps a little use in perfumery as a modifier in Oriental fragrance types, Lavender and Fougères, etc. However, one can easily be without it and very likely, most perfumers will never miss it in their daily work.

Prod.: from *n*-Heptyl bromide and Phenol in aqueous alkaline solution.

31-144;

## 1560: HEPTYL PHENYLETHYL ETHER

Phenylethyl heptyl ether.
Heptyl phenethyl ether.



$C_{15}H_{24}O = 220.36$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Powerful aromatic, warm-floral, earthy odor with some resemblance to Hyacinth and Gardenia.

Although not one of the more beautiful Phenylethyl ethers, this ether is an interesting member of that series. It has been suggested for use in perfume compositions, mainly floral, exotic-floral and in certain types of "New Mown Hay" odor, where its power can be utilized fully.

Its main drawback is probably the lack of versatility, on which point this ether is definitely inferior to most of the better known Phenylethylethers.

Prod.: from Heptanol and Phenylethyl alcohol with a dehydrating agent.

It has also been prepared from Benzyl magnesium chloride by Grignard reaction with Bromo di-heptylether.

31-144;

## 1561: HEPTYL PROPIONATE

Heptyl propanoate.

$C_7H_{15}$—OOC—$C_2H_5$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Sp.Gr. 0.87. B.P. 202° C.

Almost insoluble in water, soluble in alcohol and oils.

Ethereal-winey, but somewhat "bitter" odor, or an "astringent" odor-impression, similar to that of certain unripe fruits. Waxy-aldehydic notes appear along with a rather dry undertone.

This peculiar odorant is occasionally used in perfumes as a modifier in Fougères, Chypres and other herbaceous or floral-herbaceous fragrance types.

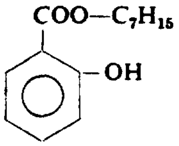
In the author's opinion, it is not a very attractive odor as such, and can only play a minor role in any type of fragrance.

Prod.: by direct esterification of *n*-Heptanol with Propionic acid under azeotropic conditions, or with Propionic anhydride.

4-60; 33-620; 35-61; 86-58;

## 1562: HEPTYL SALICYLATE

*n*-Heptyl-*ortho*-hydrobenzoate.



$C_{14}H_{20}O_3 = 236.31$

Colorless oily liquid. B.P. 300° C.
Sp.Gr. 1.03.

Insoluble in water, soluble in alcohol and oils.

Very faint, sweet-herbaceous odor. To some observers, this ester is virtually odorless.

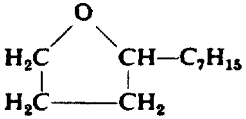
Odor descriptions often include the word "metallic", but the author of this work believes that the pure ester does not carry such odor. Traces of Phenol from the salicylic radicle may well appear as "metallic" at very low concentration in the ester, and it is not uncommon that these high-boiling esters contain traces of Phenol due to overheating, probably in an insufficient vacuum during the final distillation.

The ester has been suggested for use in perfume compositions as a modifier in Fougères and other, mainly non-floral, fragrance types where salicylates are often used. However, its odor is much weaker than that of Amyl salicylate, and not as versatile in its type.

Prod.: from *n*-Heptanol and Salicylic acid by direct esterification under azeotropic conditions.

31-130; 34-788; 35-59;

## 1563: 2-(n-HEPTYL)-TETRAHYDROFURAN



$C_{11}H_{22}O = 170.30$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Fruity-floral, quite diffusive odor. One is tempted to compare the odor to those of the Jasmone-related chemicals. But the subject ketone does not have the penetrating floral note, nor does it have the discrete fruitiness of the better Jasmone-relatives.

However, this ketone should be judged from its own performance as an individual, new material, not a substitute for an already existing series of chemicals.

In that case, there is undoubtedly interest in this rather new perfume chemical. It lends power to Fougère and Lavenders as well as it does to floral fragrance, and it is very stable towards all reasonable types of chemical reagents encountered in modern cosmetic preparations and soap.

It is still too early to predict any future of this chemical since it is barely available commercially since 1967.

Prod.: By chlorination of Tetrahydrofuran, followed by Grignard reaction with Hexyl magnesium bromide.

Also produced from Furfural.

See also: 69-163;
and: Chemical Abstracts, March 1967.

## 1564: HEPTYL UNDECENYL ETHER

Undecenyl heptylether.
(Sometimes confused with Heptyl undecylether).

$C_7H_{15}—O—CH_2(CH_2)_8CH=CH_2$

$C_{18}H_{36}O = 268.49$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Mild and fatty-floral, fruity and slightly "aldehydic" odor with some resemblance to Peach and Apricot.

Has been suggested for use in perfume compositions as a modifier for alifatic and olefinic aldehydes. It may soften the effect of the conventional aldehydes without really changing the overall character of these, but it does not contribute very interesting or unusual notes to a fragrance.

Prod.: From *n*-Heptanol and Undecylenic alcohol by dehydration.

See also: 37-176;

## 1565: HEPTYL UNDECYLATE

Heptyl undecanoate.

$C_7H_{15}—OOC—C_{10}H_{21}$

$C_{18}H_{36}O_2 = 284.49$

Colorless oily liquid. B.P. 271° C.
Sp.Gr. 0.88.

Insoluble in water, soluble in alcohol and oils.

Oily-fatty, not very pleasant odor with earthy-mossy undertones. Older odor descriptions include the words "smokey and ink-like", but the author is unable to detect any such odor type in the few available samples of subject material.

This ester has been suggested for use in perfume compositions, but although its odor type is fairly interesting, its power is negligible as compared to many common and frequently used materials. It could find some use in Cognac notes (for perfumes and for flavors) or as part of the topnote in herbaceous or citrusy fragrance types.

Prod.: by direct esterification of *n*-Heptanol with Undecylic acid under azeotropic conditions.

4-60; 31-130;

## 1566: HEPTYL UNDECYLENATE

Heptyl undecenoate.

$C_7H_{15}—OOC(CH_2)_8CH=CH_2$

$C_{18}H_{34}O_2 = 282.47$

Colorless oily liquid. B.P. 285° C.
Sp.Gr. 0.88.

Insoluble in water, soluble in alcohol and oils.

Mild, woody-fruity odor, earthy-green and with sweet-soil-like undertones, remotely resembling of notes in Vetiverol or Vetiveryl acetate.

Very rarely offered commercially, this ester has found a little use in perfume compositions as a modifier for herbaceous and woody notes in non-floral fragrance types.

Prod.: by direct esterification of *n*-Heptanol with Undecylenic acid under azeotropic conditions.

45-59; 86-58;

## 1567: HEPTYL UNDECYL ETHER

Undecyl heptyl ether.
(Sometimes confused with Heptyl undecenyl ether).

$C_7H_{15}—O—C_{11}H_{23}$

$C_{18}H_{38}O = 270.50$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Ethereal and comparatively diffusive odor reminiscent of the odor of higher alifatic aldehydes, yet with much less power.

Has been suggested for use in perfume compositions and is occasionally used in artificial essential oils and flower absolutes. Its odortype and effect in general are, however, not very unusual or powerful or outstanding.

Prod.: from *n*-Heptanol and Undecylic alcohol by dehydration.

31-144; 37-176;

## 1568: HEPTYL VALERATE

*n*-Heptyl-*n*-pentanoate.
Heptyl valerianate.

$C_7H_{15}—OOC—(CH_2)_3CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. B.P. 243° C. Sp.Gr. 0.88.

Insoluble in water, soluble in alcohol and oils.

Peculiar fruity odor with a woody-animal-like undertone, even when no trace of Valeric acid seems to be perceptible.

The ester has been suggested for use in perfume compositions where Civet-notes are applied, or in making artificial Civet, etc. It will also give useful effects in Men's fragrances of Leather or "Tabac" type. The ester blends well with Lavender, Clary Sage and most other non-floral natural materials, and Styrax makes a suitable fixative for the ester.

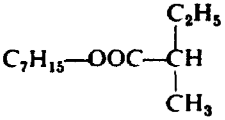
In flavors it has been used for imitation Apple and in tobacco flavorings, but it is not powerful enough to become very interesting as an Apple item, and it is not "natural" enough in its Aroma to be an attractive item for Tobacco.

Prod.: by esterification of *n*-Heptanol with *n*-Valeric acid under azeotropic conditions.

4-60; 7-205; 86-58;

## 1569: HEPTYL-iso-VALERATE

Heptyl methyl ethyl acetate.
Heptyl-*iso*-pentanoate.



$C_7H_{15}—OOC—CH(C_2H_5)(CH_3)$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Sp.Gr. 0.87. B.P. 235° C.

Insoluble in water, soluble in alcohol and oils.

Green-fruity, rather fresh and "juicy" odor resembling that of freshly crushed unripe fruit (e. g. Gooseberry) with an undertone like wet grass.

This ester has been suggested for use in perfume compositions, mainly as part of topnote complexes for Violet fragrances, where it may round off the sharper notes of Acetylenic esters or olefinic alcohols, and add a pleasant freshness to the composition.

It could possibly find use in flavor compositions, such as imitation Apple, Gooseberry, Guava, Rhubarb and other comparatively rare and unusual flavor types in which the green notes lean toward the "unripe" and "juicy" side.

The ester is NOT listed in the American Federal Register as G.R.A.S.

Prod.: by direct esterification of *n*-Heptanol with *iso*-Valeric acid under azeotropic conditions.

4-59; 33-932; 35-61; 103-123;

## 1570: HERCOLYN

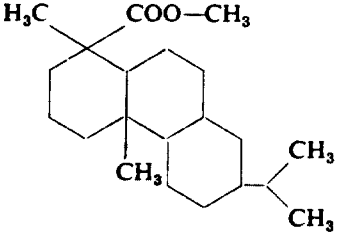
Not a well-defined chemical.

The commercial product under subject name consists of the Methylesters of hydrogenated rosin acids, mainly:

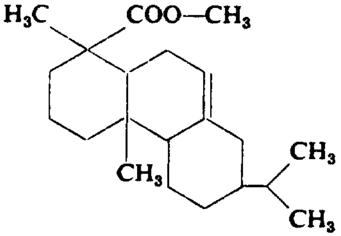
A) Tetrahydro methylabietate and

B) Dihydro methylabietate.

HERCOLYN D is a specially deodorised quality of Hercolyn.



A) $C_{21}H_{36}O_2 = 320.52$



B) $C_{21}H_{34}O_2 = 318.50$

B.P. approximately 366° C. Sp.Gr. 1.03.

Very viscous, but pourable pale straw-colored or very pale amber-colored liquid. Insoluble in water, soluble in alcohol and oils.

Hercolyn D is almost odorless when freshly prepared and properly stored, but it will easily take odors from other chemicals if exposed to their vapors.

Regular Hercolyn has a faint, woody-piney odor of considerable tenacity. Hercolyn D is the most commonly used in perfumery, where the material finds application as a blender-fixative in many types of low-cost fragrance, particularly those designed for household products and for industrial purposes. It is particularly suitable for pine odors, but it can be used in modest amounts in most non-floral and a few floral fragrance types.

The excessive use of Hercolyn, e. g. as a diluent, may not alter the odor of a pine fragrance very much, but it may cause some problems in the solubility of the fragrance, or its compatibility with certain cosmetic raw materials in the functional product. And in the more delicate floral fragrances, e. g. the conventional "Appleblossom" type for many household products, there is a distinct limit to the amount of Hercolyn to be used without a perceptible change of the fragrance. The woody-piney notes of Hercolyn are particularly conspicuous .in such florals or delicate fragrance types. In all, Hercolyn is one of the most useful blenders for low-cost fragrances, and it is, in many cases, a better fixative than Diethylphthalate.

Prod.: By Methyl-esterification of the hydrogenated acids from American Turpentine rosin.

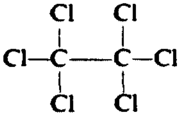
86-58; 86-61;

sample: Hercules Powder Co. Also data sheet.

See also: Abitol – and Methyl abietate.

## 1571: HEXACHLOROETHANE

Perchloroethane.
Carbon hexachloride.



$\mathrm{Cl_3C{-}CCl_3}$

$C_2Cl_6 = 236.76$

Colorless crystals. Sp.Gr. 2.1. Sublimes (before melting) at 187° C.

Insoluble in water, soluble in alcohol and oils.

Mild Camphor-like odor of moderate tenacity, and not as "medicinal" as Camphor.

This chemical has been used in place of Camphor in the manufacture of Celluloid. It is also a moth repellant with somewhat better effect than Camphor.

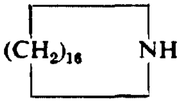
Although it is not truly a fragrance material, it may occasionally find use as a substitute for Camphor in industrial odors, e. g. when Camphor prices are high.

Prod.:

1) by chlorination of Acetylene tetrachloride in sunlight or in the presence of Aluminum chloride.
2) by heating Carbon tetrachloride with Aluminum amalgam.

66-278; 100-514; 160-974; 1-255;

## 1572: HEXADECAMETHYLENIMINE



$C_{16}H_{33}N = 239.45$

Colorless viscous oil.

Insoluble in water, soluble in alcohol and oils.

Faint, sweet-musky odor of excellent tenacity.

Has been suggested as a fixative with mild musky effect for perfume compositions. However, this material is inferior to many better known and commercially available macrocyclic musks with respect to power and chemical stability, and it is most conceivable that subject material will remain on the research shelf and enjoy only academic interest.

Prod.: from Pentadecamethylene ketone via the Oxime and *iso*-Oxime to the Thiosoxime. The latter is reduced to the subject Imine.

30-275; 31-103; 156-265;

## 1573: HEXADECANAL

Hexadecyl aldehyde.
Palmitic aldehyde.
Palmitaldehyde.
Aldehyde C-16 (true).

$CH_3(CH_2)_{14}CHO$

$C_{16}H_{32}O = 240.43$

Solid white or colorless waxy mass.

M.P. 34° C. Liquid is a colorless oil.
B.P. 310° C.

Insoluble in water, soluble in alcohol and oils.

Weak and mildly floral, orrisy-waxy odor. Some observers describe the odor as "peachy", but the author of this work fails to find any such note in subject material.

By and large of little or no use to the perfumer, there is yet one application for which this aldehyde seems to be quite suitable: for artificial Mimosa absolute, or in "Mimosa" bases. The choice of materials truly suitable for Mimosa bases is extremely small, and any material which has a useful effect should be very welcome. This special application may also lead to the use of Hexadecanal in other floral fragrances or bases, e. g. Tuberose, Cassie, Peony, etc. and the aldehyde blends very well with the Ionones in an artificial Cassie composition.

Prod.: by catalytic reduction of Hexadecanol (Cetyl alcohol).

4-60; 7-206; 36-1029; 89-35;

## 1574: HEXADECANOL

Cetyl alcohol.
*alpha*-Oxy-hexadecane.
*l*-Hexadecanol, *primary*.
Alcohol C-16.
Palmityl alcohol.
Ethal.
*n*-Hexadecyl alcohol.
"Lorol No. 24" (DuPont) is mainly
Hexadecanol.
(See note below).

$CH_3(CH_2)_{14}CH_2OH$

$C_{16}H_{34}O = 242.45$

Snow-white or colorless leafy crystals.
M.P. 50° C. Sp.Gr. 0.81 (liquid).
B.P. 344° C.

Insoluble in water, 50% soluble in alcohol, miscible with most oils.

The pure material is virtually odorless. Lower grade commercial products may have a faint, sweet, oily odor and a bland taste.

Although very extensively used as a cosmetic raw material (for creams, etc.), this alcohol is rarely, if ever, used in perfumes as a fragrance material.

It finds some use in flavor compositions in minute traces in imitation chocolate flavors, mainly to introduce a mouthfeel, rather than a taste. The concentration used is about 2 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2554.

Prod.: by alcoholic saponification of the Palmitic ester of Hexadecanol (Spermaceti from the Whale is almost pure Cetyl palmitate).

4-30; 66-314; 100-227; B-I-429; 155-285; 155-286;

NOTE: The name Hexadecylalcohol is also used for a liquid $C_{16}$ alcohol of branched chain structure.

That alcohol is used exclusively as a cosmetic emollient, harmless to the human skin.

## 1575: 2,4-HEXADIENAL

Sorbic aldehyde.
*2*-Propylene acrolein.

$CH_3—CH=CH—CH=CH—CHO$

$C_6H_8O = 96.13$

Colorless liquid. B.P. 174° C. Sp.Gr. 0.91.

Almost insoluble in water, soluble in alcohol and oils.

Powerful but sweet-green odor, in dilution pleasant citrusy-fresh-green, in high concentration rather pungent, choking. Poor tenacity. The aldehyde is severely affected by contact with air, and it changes odor and viscosity very rapidly if exposed to air, daylight, or heat, e. g. if improperly stored.

This aldehyde, simple as it is, remains half-secret and is rarely, if ever, found on the shelves in the perfume laboratories. When freshly prepared, it has a very attractive odor, and, being a diene aldehyde, it shows strong tendency to polymerization, wherefore it keeps much better in dilution or – as a minor component in a base. And this is where it is mostly found: as part of fresh topnote bases, not only citrusy types, but many floral or green types, too.

It blends very well with Citral, Myrac aldehyde, the Hexenols and their derivatives, Citrus oils, Citronellol, Galbanum, etc., and once it is incorporated and well diluted, it shows much less tendency of deterioration.

Prod.:

1) from Acetaldehyde, by self-condensation (3 mols.)
2) from Acetaldehyde by condensation with Croton aldehyde.

Sorbic aldehyde is an industrial chemical available in large volume. It is also used in the manufacture of Sorbic alcohol.

66-504;

## 1576: HEXADIENE

Biallyl.
Diallyl.
*1,5*-Hexadiene.

$CH_2{=}CH{-}CH_2{-}CH_2{-}CH{=}CH_2$

$C_6H_{10} = 82.15$

Almost colorless mobile liquid. Sp.Gr. 0.69. B.P. 60° C.

Insoluble in water, somewhat soluble in alcohol, miscible with most oils.

Powerful, diffusive, sweet, somewhat gassy-green, but not really unpleasant odor of very poor tenacity.

Although not a fragrance material as such, this hydrocarbon may occasionally be used as part of industrial masking odors, and it may also appear as an impurity in various perfume chemicals.

Prod.: from Allylbromide and Sodium (or Magnesium).

31-4; 66-270; 160-1032;

## 1577: HEXADIENOL

*2,4*-Hexadien-*1*-ol.
Sorbyl alcohol.
Sorbic alcohol.
*1*-Hydroxy-*2,4*-hexadiene.
Hexakose.

$CH_3{-}CH{=}CH{-}CH{=}CH{-}CH_2OH$

$C_6H_{10}O = 98.15$

Colorless or white needle-like crystals.
M.P. 31° C. B.P. 177° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-oily, green odor, somewhat grassy-weedy, but quite refreshing and moderately tenacious. The alcohol oxidizes very easily in air and this process affects the odor considerably to the disadvantage of the pleasantness of this alcohol.

This conjugated diene alcohol is occasionally used in perfume compositions as part of a "green note", mostly for topnote effects in Muguet or Lily, but also in various non-floral types.

Its sensitivity to air oxidation is a severe drawback and it is most likely that the use of this alcohol will be abandoned since the last decade has brought us so many excellent and stable, natural green odorants, particularly those of the Hexenyl family.

Prod.:

1) by Ponndorf reduction (with Aluminum-*iso*-propoxide in *iso*-Propanol solution) of the corresponding aldehyde, Hexadienal.
2) the alcohol can also be obtained by reduction of the Ethyl ester of the acid, Sorbic acid, which is prepared from Croton aldehyde by Malonic acid condensation.

66-319; 100-968;

## 1578: HEXADIENYL-iso-BUTYRATE

Sorbyl-*iso*-butyrate.

$CH_3{-}CH{=}CH{-}CH{=}CH{-}CH_2{-}OOC{-}CH(CH_3)_2$

$C_{10}H_{16}O_2 = 168.24$

Colorless or very pale straw-colored liquid.

Almost insoluble in water, soluble in alcohol and oils.

Oily-sweet, fruity-green, Apple- and Galbanum-like odor with more sweetness and fruitiness than Galbanum, and overall more fruity than green notes. Fair tenacity.

The taste is sweet, green-fruity, mainly Apple-like.

This ester, not often offered commercially, is surprisingly stable and its natural odor can be very useful in many perfume compositions.

It performs well with the Citrus oils, and it gives interesting effects with Undecanolide, which has had a come-back along with Methylnonyl acetaldehyde in "new fragrance notes". It will take the overly sweet-fruity and rather heavy tone out of Undecanolide and at the same time soften the dry notes of the aldehyde.

Hexadienyl-*iso*-butyrate is also used in flavor compositions (outside of the U.S.A., since it is NOT listed as a G.R.A.S. material). It produces very pleasant effects in Apricot, Apple, Mango and Peach imitation flavors.

Prod.: by direct esterification of Hexadienol with *iso*-Butyric acid under azeotropic conditions.

## 1579: HEXADIENYLIDENE ACETONE

*3,5,7*-Nonatrien-*2*-one.

$$CH_3—CH{=}CH—CH{=}CH—CH{=}CH—CO—CH_3$$

$$C_9H_{12}O = 136.20$$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-oily, citrusy and refreshing, green odor of moderate tenacity. Undiluted not very pleasant, rather oily-fatty, but at concentrations near 1 %, or in proper composition, the odor appears more citrusy, sweeter, fresher.

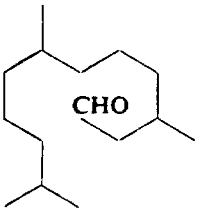
This relatively simple, but commercially rare item finds use in perfume compositions as an important part of certain topnote specialties, bases, etc. It is mainly used in the citrusy type, but also in the so-called "aldehydic" base, which is normally a composition of alifatic aldehydes, delicately green notes, fruity notes, and a rich, but delicate floral note, often Muguet. This type base has been used conventionally in modifications (or "copies") of very many successful luxury perfumes, including several great names.

The title aldehyde is rarely, if ever, offered for sale as such, but it is not difficult to prepare, It is also comparatively inexpensive, but it deteriorates easily unless diluted or well protected. Therefore, there is one more reason to handle the aldehyde in compositions only, where the dilution provides sufficient protection for the aldehyde.

Prod.: by condensation of Sorbic aldehyde and Acetone (Claisen condensation).

## 1580: HEXAHYDROFARNESAL

*2,6,10*-Trimethyl dodecanal.



$$C_{15}H_{30}O = 226.41$$

Almost colorless or pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant, sweet-rosy, citrusy odor, less floral than Trimethyl undecanal (known as Norhexahydro farnesal) and Tetrahydro farnesal. Very tenacious and waxy-petal-like.

This aldehyde finds some use in perfume compositions although the related aldehydes, many of which are known under a wealth of trade names, are generally superior in one aspect or the other. The subject aldehyde may be superior in citrusy sweetness, and somewhat less fatty, but it does not have the enormous power and amplitude of some of the unsaturated relatives.

It is often necessary to work with concentrations of less than one percent in order to prevent this peculiar note from dominating the fragrance.

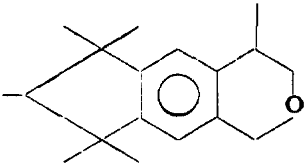
Prod.:

1) by hydrogenation of Farnesol with Raney-Nickel catalyst, followed by oxidation to the subject aldehyde.
2) from Nerolidol via oxidation to Farnesal which is hydrogenated to subject aldehyde.

2-1018; 88-237; 88-238; 89-125;
see also: 31-39; and R. W. Moncrieff in Soap, Perfumery and Cosmetics, vol. 22, 1949, page 1106.

## 1581: 1,3,4,6,7,8-HEXAHYDRO-4,6,6,7,8,8-HEXAMETHYL-CYCLOPENTA-gamma-2-BENZOPYRAN

An Indan-type *iso*-Chroman Musk.
"Galoxolide" (I.F.F.).



$C_{18}H_{26}O = 258.41$

Almost colorless, very viscous liquid. The commercial product is sold in a diluted state in order to make the material handy and pourable at room temperature.

Insoluble in water, soluble in alcohol and oils.

Sweet and musky odor of good tenacity, comparable to that of many related products, but much inferior to the tenacity of the modern macrocyclic Lactone type Musks. Similar to many Indan and Tetralin Musks, it has a tendency of appearing somewhat woody and not sufficiently sweet.

Increasingly used in perfume compositions, it has become popular as one of the lowest priced Musks of this chemical group.

The woody-musty, root-like notes at higher concentration are usually overcome by the simultaneous use of sweeteners, such as Undecanolide, Cinnamates, Balsams, etc.

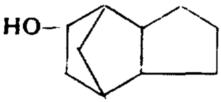
Due to character of the diluent, this Musk is NOT recommended for flavors.

Prod.: from Pentamethyl indan.

156-287;

## 1582: 3a,4,5,6,7,7a-HEXAHYDRO-4,7-METHANO-5-INDANOL

Tetrahydro-6-Hydroxy dicyclopentadiene.



$C_{10}H_{16}O = 152.24$

Semi-solid, crystalline mass, or viscous, pale straw-colored or almost colorless liquid, solidifying in the cold.

Practically insoluble in water, soluble in alcohol and oils.

Peculiar earthy-sweet, musty odor of moderate tenacity.

This alcohol, related to the Hydroindols (see monograph), has been developed since the Cyclopentadiene and its derivatives became available as very low cost industrial chemicals, mainly intended for large-scale industrial exploitation of the Diels-Alder synthesis.

A number of adducts and derivatives have been made, and a few have become useful perfume chemicals.

The title material has notes in common with Sandalwood, Oakmoss, Cedarwood and Galbanum, and it could be used in conjunction with such naturals. It is stable in soap and offers a low-cost material for soap, detergent and other household product fragrances. Its musty character blends well with woody and Ambre-like notes, but leaves a floral picture out of the question.

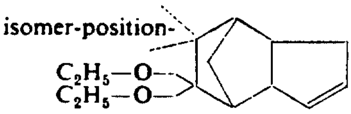
The title material is rarely offered under its chemical name, but it may enter various specialties and perfume bases as a minor component. During the 1965-66 period of scarcity and high prices of Patchouli oil, the subject alcohol found some use in the creation of Patchouli oil substitutes.

See also U.S. patent No. 3.271.259 (Oct. 22, 1965) of Harry Saunders, U.O.P. Chem. Co. The above material is a parent of various Lavandin-substitute Aroma-chemicals.

## **1583:** 3a,4,5,6,7,7a-**HEXAHYDRO**-4,7-**METHANOINDENE**-5-**CARBOXALDEHYDE DIETHYLACETAL**

The diethylacetal of Dihydrocyclopentadiene *5*- or *6*-aldehyde.

The commercial product usually contains a mixture of at least two isomers.



$C_{14}H_{23}O_2$ = 223.34

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet and herbaceous-winey odor with Basil-Neroli-like notes and good tenacity. The commercial material is not absolutely pure, and may well display traces of "celluloid"-like notes, but these are rarely perceptible when the material is incorporated in a composition.

This peculiar perfume chemical has exceptional versatility in application – from Orangeblossom to herbaceous and spicy, from sophisticated Pine needle to delicately floral.

It is therefore an excellent material for new versions of the ever-popular Chypre theme, where Orangeblossom may be combined with sweet-herbaceous notes through Oakmoss and precious woods, and where Basil notes are certainly at home.

The acetal is not offered under its proper chemical name (who could ever remember it anyway!) but it finds its way into various specialties under trade names.

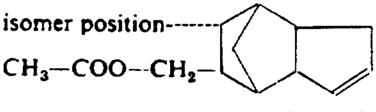
Prod.: from Dihydro dicyclopentadiene aldehyde with Ethyl-*ortho*-formate in presence of a mineral acid catalyst.

## **1584:** 3a,4,5,6,7,7a-**HEXAHYDRO**-4,7-**METHANOINDENE**-5-**METHYLACETATE**

The acetate of Dihydrocyclopentadiene *5*- or *6*-methanol.

A further development of Cyclol and Cyclyl acetate (see that monograph).

The commercial product usually consists of a mixture of isomers.



$C_{13}H_{18}O_2$ = 206.29

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

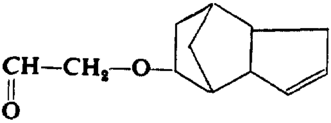
Mild and sweet fruity-woody odor of moderate tenacity. The fruity notes are without specific character, and the overall impression is that of a rather chemical odor. Except for its low cost and relative ease of manufacture, this ester does not offer any significant advantage over similar-smelling chemicals.

It has been used as a low-cost edition of Linalyl acetate, and as a modifier for *iso*-Bornylacetate, mainly in detergent and soap perfumes, etc., but it is, to the author's knowledge, no longer commonly used.

Prod.: from Chloro dihydro dicyclopentadiene with Magnesium and Ethylformate.

## 1585: 3a,4,5,6,7,7a-HEXAHYDRO-4,7-METHANOINDEN-5-YL OXYACETALDEHYDE

The Oxyacetaldehyde of *5*- or *6*-Hydroxy Dihydro dicyclopentadiene.
The commercial material may consist of a mixture of isomers.



$C_{12}H_{16}O_2 = 192.26$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet, green-floral and somewhat woody-earthy odor of good tenacity.

This aldehyde has found use in perfume compositions as a minor component in green-floral and delicately sweet floral fragrance types. It blends very well with the Lilac, Hyacinth and Narcisse-materials, the "rose alcohols" etc., and it gives pleasant variations with Cyclamal and Lilial (Bucinal).

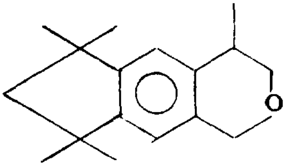
The Hexenals may be added in trace amounts to this aldehyde to lend more natural greenness, and to increase the power for use in soap perfumes.

The title aldehyde is not offered under its chemical name, but it has been available under various trade names and as component of various specialties.

Prod.: from Dicyclopentadiene alcohol with Monochloroacetaldehydedimethylacetal and a Sodium metal catalyst. The resulting acetal is hydrolyzed under acid conditions to free the subject aldehyde.

## 1586: 1,3,4,6,7,8-HEXAHYDRO-4,6,6,8,8-PENTAMETHYL-CYCLOPENTA-gamma-2-BENZOPYRAN

An *iso*-Chroman Musk.



$C_{17}H_{24}O = 244.38$

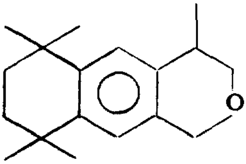
This Musk, which is the next lower homologue of the previously described material (see monograph No. 1581) may be considered as practically obsolete. It is comparatively new (1961-64) but has been by-passed in the competition with more recently developed, lower priced and better performing Musks.

Apart from having a typical Musk odor and good tenacity, it does not offer any effects that can justify its preference over the newer, related materials.

See also: 156-287;

## 1587: 3,4,6,7,8,9-HEXAHYDRO-4,6,6,9,9-PENTAMETHYL-1H-NAPHTO-(2,3,c)-PYRAN

An *iso*-Chroman type Musk, Tetralin type.



$C_{18}H_{26}O = 258.41$

Viscous, almost colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and musky odor of good tenacity, but not quite as powerful as the isomer of Indan type (see monograph No. 1581).

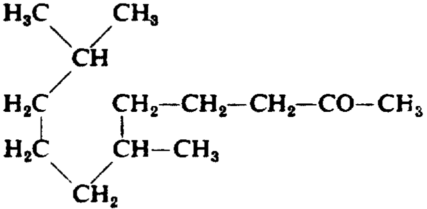
Has been suggested for use in perfume compositions as a musk-fixative of good stability and little or no tendency of discoloration in soap. However, this material was developed in the years of extremely fast discoveries of new musks, and it may already be considered as more or less obsolete, unless it could be produced at a much lower cost, which would undoubtedly re-create some interest in the material.

Produced from *iso*-Chroman.

See also: 156-287;

## 1588: HEXAHYDRO PSEUDOIONONE

*6,10*-Dimethyl undecan-*2*-one.



$C_{13}H_{26}O = 198.35$

Almost colorless, slightly oily liquid.
Sp.Gr. 0.84.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, herbaceous-floral, somewhat woody odor of moderate tenacity. The floral notes tend to appear rosy, the herbaceous sweetness is almost haylike/Lavender-like, and the undertones are also fruity.

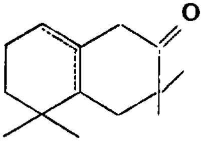
This material, often sold under trade names, is used in perfume compositions as a modifier in low-cost Rose formulations, mainly for household product fragrances, etc. It may introduce a freshness resembling that obtained from Norhexahydrofarnesal, but it does not have the power of that aldehyde. It blends excellently with Citrus materials, "Rose alcohols", Cedarwood derivatives, Lavandin and other herbaceous oils, etc.

Prod.: by complete hydrogenation of Pseudo ionone, e. g. by Ponndorf reaction (Aluminum *iso*-propoxide reduction).

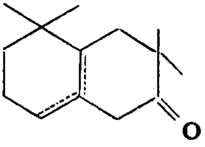
4-60; (also: Givaudan Corp. data sheet and info.).

## 1589: HEXAHYDRO TETRAMETHYL NAPHTHALENONE

Tetramethyl-*beta*-hexalone.
The monograph includes the isomers, usually accompanying the title material.



and:



$C_{14}H_{23}O = 207.34$

Colorless or very pale straw-colored viscous liquid, usually separating crystals, and solidifying in the cold to an opaque crystalline mass, depending upon the isomer-ratio in the product.

Insoluble in water, soluble in alcohol and oils.

Camphoraceous-musky, but also musty odor of considerable tenacity. Woody notes and degree of camphoraceous topnote seems to vary with the isomer ratio. Undoubtedly, the sweet-musky, precious-wood-like notes are the preferred portion of the mixture, but the product does not seem to be marketed as a single, isolated chemical.

This product has been suggested for use in perfume compositions, mainly as a fixative/blender/modifier in woody-musky compositions, particularly in soap perfumes, etc.

It blends very well with Indane-type musks, Sandalwood, Cedarwood derivatives, Ionones, etc. but it is most conceivable that the material will fall into oblivion if it cannot be manufactured in a reproducible quality, preferably in the form of the isolated, purified, olfactorily superior isomer.

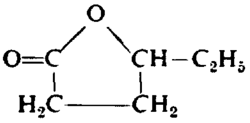
For those interested in the study of odor and chemical structure, it may be of interest to compare this item to Fixateur 404 and its higher homologue – see monographs. Long before the true Ambergris products (Fixateur 404 and related chemicals) were brought into the market, the perfume chemists had their attention concentrated upon certain derivatives of Hexalin and Decalin. The author would predict that these materials have served their purpose as intermediate helpers until we could have the true Ambergris chemicals commercially available. It is also interesting to compare the structure of this material to those of "Versalide", "Tonalid", etc. – see monographs:

*4*-Acetyl-*1,1*-dimethyl-*6*-*tertiary*-butylindan, (Celestolide, IFF),
*6*-Acetyl-*1,1,3,4,4,6*-hexamethyl tetrahydronaphthalene (Tonalid, PFW),
*5*-Acetyl-*1,1,2,3,3,6*-hexamethyl indan (Phantolid, PFW),
Versalide (Givaudan).

And it is furthermore interesting to study the similarity to the structure of Abietic acid – see monograph "Abitol", which in turn has much in common with the structure of Manool – see monograph.

## 1590: gamma-HEXALACTONE

Hexanolide-*1,4*.
*gamma*-Ethyl-*n*-butyrolactone.
Tonkalide.



$C_6H_{10}O_2 = 114.15$

Colorless liquid. Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Warm, powerfully herbaceous, sweet "Tobacco-like", coumarinic type odor.

Sweet, powerful, warm-herbaceous, Coumarin-Caramel taste.

This Lactone finds some use in perfume compositions as a modifier for Coumarin, in Lavender and Fougère perfumes, and in many other types where Oakmoss is used as a sweetener for mossy notes.

This material is more widely used in flavors, where its power and creamy sweetness is utilized for imitation Butter, Honey, Vanilla, Caramel and in fruit complexes and Tobacco flavorings.

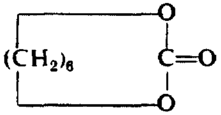
The concentration used may vary from 0.1 ppm to 20 ppm in most of the common finished products, except in ice cream where it may be as high as 60 to 90 ppm.

It performs very well with Vanillin as a synergist for the Vanilla and Cream-like flavor, an effect previously supplied by Coumarin.

Prod.: (many methods) e. g.: from Ethylene oxide and Sodio-malonic ester. Also from Propyl alcohol and Methylacrylate in presence of Di-*tertiary*-butyl peroxide catalyst.

G.R.A.S. F.E.M.A. No.2556.

## 1591: HEXAMETHYLENE CARBOXYLATE



$C_7H_{12}O_3 = 144.17$

Subject chemical, of very little interest beyond that of the academic, represents one of the lowest members of a series of fairly interesting perfume chemicals. Higher members may have Musk odors (Undecamethylene- and higher) and a few of these have found enough interest to become commercially developed.

The subject ester however, has only a rough minty-camphoraceous odor, somewhat reminiscent of Pennyroyal oil, and the ester could find some use as a material for masking odors for industrial purposes.

Prod.: from Hexamethylene glycol and Butyl carbonate with Sodium catalyst, followed by depolymerization of the Polyester. It has also been prepared from Hexamethylene glycol and Phosgene (Carbonyl chloride).

31-127; see also: 66-681;

## 1592: n-HEXANAL

Caproaldehyde.
Caproic aldehyde.
Aldehyde C-6.
Hexyl aldehyde.
Hexoic aldehyde.
Hexaldehyde.

$CH_3(CH_2)_4CHO$

$C_6H_{12}O = 100.16$

Colorless mobile liquid. Sp.Gr. 0.82.
B.P. 131° C.

Almost insoluble in water, miscible with alcohol, Propylene glycol and oils.

Very powerful, penetrating, fatty-green, grassy odor. In extreme dilution more reminiscent of freshly cut grass and unripe fruits (Apple and Plum). The acrid note of the concentrated material resembles that of rancid Butter.

The aldehyde is easily oxidized in air to Caproic acid which is mainly responsible for the "rancid" notes.

This aldehyde is occasionally used – in very disrete amounts – in perfumes as part of a top-note complex, or in the reproduction of artificial essential oils, etc. As a "green" odor, it does not give the naturalness or beauty of the unsaturated aldehydes and the corresponding alcohols and esters, but it has some advantage in a very low cost, making it useful in masking odors for industrial purposes, etc.

It is used more commonly in flavor compositions for imitation Butter, Cheese, Honey, Rum, Arak, etc. and in many fruit complexes. The concentration is normally mere traces, e. g. 1 to 5 ppm in the finished product.

NOTE: Hexaldehyde is flammable and represents a fire hazard.

Prod.: by catalytic oxidation of *n*-Hexanol (a petrochemical).

G.R.A.S. F.E.M.A. No.2557.

66-477; 89-20; 100-205; 160-900; 86-59; 4-61; (Givaudan Corp., data sheet).

## 1593: HEXANAL DIETHYLACETAL

Hexaldehyde diethylacetal.
Caproic aldehyde diethylacetal.

$CH_3(CH_2)_4CH(OC_2H_5)_2$

$C_{10}H_{22}O_2 = 174.29$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Oily-green, rather mild, grassy odor of fair tenacity. The odor is strongly influenced by the presence (or absence) of free aldehyde.

This acetal has been suggested for use in perfumes and flavors as a modification of the aldehyde, when the latter seems too pungent for the intended purpose.

However, the odor type is quite different, and the acetal can – in the author's opinion – not substitute or partly replace the aldehyde in an already established formulation.

In flavors, the acetal may also face a partial decomposition in functional products which are often acid in character, while the acetal is fairly stable in moderately alkaline media (soap, etc.).

It is therefore most conceivable, that this acetal – and related acetals – will find very little use in perfumes and flavors.

Prod.: from Hexyl aldehyde and Ethanol by condensation in presence of a dehydrating agent.

4-61;

## 1594: HEXANAL DIMETHYLACETAL

Hexaldehyde dimethyl acetal.

$CH_3(CH_2)_4CH(OCH_3)_2$

$C_8H_{18}O_2 = 146.23$

Colorless liquid. B.P. 145° C.

Almost insoluble in water (decomposes slowly), soluble in alcohol and oils.

Peculiar dry-musty, leafy-green, but overall mild and rather sweet odor. Traces of free aldehyde will naturally change the odor picture significantly.

Odor descriptions of this acetal vary considerably, some include the term "Fenchyl acetate-like", and it is apparent that the acetal has been available in various grades of odor quality.

Its poor stability and the fact that its own odor is very difficult to utilize and maintain, are factors contributing to the lack of interest in such acetals (see also previous monograph).

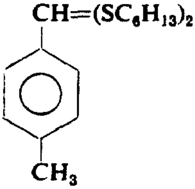
Prod.: From Hexyl aldehyde with Methanol in presence of a dehydrating agent, e. g. small amounts of dry hydrogen chloride.

86-59;

## 1595: HEXANE METHYLTHIONAL

A confusing name for the condensation product of Methylbenzaldehyde and Hexylmercaptan.

"Tolyl mercaptal".
"Hexane methyl benzyl thional".
*para*-Methylbenzaldehyde-di-*n*-hexathienyl-acetal.



$C_{20}H_{34}S_2 = 338.62$

NOTE: Commercial grade "Methylbenzaldehyde" is normally a mixture of mainly *para*-isomer with considerable amounts of *ortho*- and *meta*-isomers. The above structure describes the main component of the subject condensation product.

Pale yellowish oily liquid. Almost insoluble in water, soluble in alcohol and oils.

Extremely powerful "burnt"-alliaceous- sulfuraceous odor. In dilution the odor becomes less repulsive, and shows resemblance to the odor of freshly roasted Coffee or Cocoa beans, still with some Onion-like character.

The taste in dilutions below 2 ppm is burnt-caramellic, remotely reminiscent of Coffee.

This material, which is not a well-defined chemical, is used as a fortifier in Coffee and Chocolate flavor compositions. The concentration used is normally equivalent to 0.1 to 1.0 ppm, in exceptional cases somewhat higher.

The author is not aware of any significant use of this material in perfume compositions.

Prod.: by condensation of Tolyl aldehyde and Hexylmercaptan (*n*-Hexanethiol) using a trace of Hydrochloric acid as starter catalyst. One published process reports that the ratio of Tolylaldehyde to Hexylmercaptan should be 60/70. The theoretical proportion is 60/118, but it is undoubtedly wise to use a surplus of the sweetest smelling component.

161-212;

## 1596: HEXANOIC ACID

Caproic acid.
Hexylic acid.
*n*-Hexoic acid.
Pentane-*l*-carboxylic acid.

$CH_3(CH_2)_4COOH$

$C_6H_{12}O_2 = 116.16$

Colorless oily liquid. Solidifies in the cold, melts at minus 3° C. B.P. 205° C.
Sp.Gr. 0.93.

1 % soluble in water, miscible with alcohol and oils.

Heavy, acrid-acid, fatty-rancid odor, often described as "sweat-like".

Apart from rare occasions of use in artificial essential oils, flower absolutes, Civet bases, ets. this acid finds very little use in perfumery.

It is used in flavor compositions, mainly in Butter imitations, Butterscotch, Chocolate, Cheese, Pecan, Rum and various fruit complexes. The concentration used is normally about 2 to 30 ppm in the finished product but may be up to 450 ppm in chewing gum.

Prod.:

1) from Castor oil by Nitric-sulfuric cracking.
2) as a by-product in the saponification of Coconut oil.

G.R.A.S. F.E.M.A. No.2559.

26-448; 66-564; 90-79; 100-205; 160-900; B-II-321;

## 1597: HEXANOL

*1*-Hexanol.
*n*-Hexyl alcohol.
*n*-Amyl carbinol.
Alcohol C-6.
Caproic alcohol.

$CH_3(CH_2)_4CH_2OH$

$C_6H_{14}O = 102.18$

Colorless liquid. Sp.Gr. 0.82. B.P. 157° C.

0.6% soluble in water, miscible with alcohol, Propylene glycol and oils.

Somewhat "chemical"-winey, slightly fatty and fruity odor, weaker than Amyl alcohol, but resembling that material, except that Hexanol seems fattier and fruitier.

This alcohol finds a little use in perfume compositions, mostly in bases, artificial essential oils (geranium, etc.) and as part of various topnote-complexes. It may participate in notes giving impression of an "aged" fragrance with its winey-fermented nuances, and it helps conceal the initial, sharp notes from alcohol in perfume solutions.

Hexyl alcohol is used in flavor compositions, usually at very low concentration, in imitation Coconut, in Berry complexes and in various fruit flavors. The concentration in the finished product may be about 0.2 up to 25 ppm.

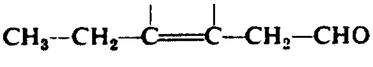
Prod.: by reduction of Ethyl caproate with Sodium alcoholate. It is also available as a petrochemical.

G.R.A.S. F.E.M.A. No.2567.

4-61; 26-572; 31-15; 66-313; 86-59; 87-465; 100-517; 160-1034; B-I-407; 140-124;

## 1598: cis-3-HEXENAL

"Leaf aldehyde" (see also *trans-2*-Hexenal).
*beta-gamma*-Hexylenic aldehyde.



$CH_3-CH_2-\overset{H}{\overset{|}{C}}=\overset{H}{\overset{|}{C}}-CH_2-CHO$

$C_6H_{10}O = 98.15$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. Fairly soluble in Propylene glycol.

Powerful, deep-green, leafy odor reminiscent of Strawberry-leaf and wine-leaf, freshly crushed.

This aldehyde is occasionally used in perfume compositions as part of a "green" topnote complex, not only for herbaceous fragrance types, but also in various floral compositions. The concentration will normally be less than 0.1 percent in the perfume oil.

It should be kept in mind, that solutions of this aldehyde – and many related aldehydes – in Ethylalcohol, Propyleneglycol and several other alcohols, may result in the formation of Acetals of odor types entirely different from those of the parent aldehydes. It is therefore safer to use Diethylphthalate as diluent for these aldehydes in work with perfumes. For flavors, freshly prepared dilutions in alcohols can be used.

The subject aldehyde is used in flavor compositions in minute traces to introduce a natural, green note in many types of fruit flavor. Concentrations in the finished product may be about 0.2 to 5 ppm.

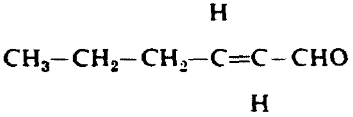
Prod.: by oxidation of Hexenol.

G.R.A.S. F.E.M.A. No.2561.

31-50; 34-1210; 156-25;

## 1599: trans-2-HEXENAL

*beta*-Propyl acrolein.
*alpha-beta*-Hexylenic aldehyde.
*2*-Hexenal.
"Leaf aldehyde" (sometimes called – see also *cis-3*-Hexenal).



$$CH_3-CH_2-CH_2-\overset{H}{C}=\underset{H}{C}-CHO$$

$C_6H_{10}O = 98.15$

Colorless liquid.

Almost insoluble in water, soluble in alcohol, Propylene glycol and most perfume and flavor oils.

Powerful green-fruity, pungent vegetable-like odor, pungent in high concentrations, almost acrylic-sharp, but pleasant fruity and fresh-green in dilutions below 0.1 %.

Used in perfume compositions as part of fresh-green, natural topnote complexes, often in delicately floral or fruity fragrance types, and in general as a fresh topnote in bases and artificial essential oils. It performs very well with the overly sweet notes of Ethyl Methyl Phenyl Glycidate or Undecanolide, and in minute traces with Palatone or Ethyl Veltol (also in minute traces), it may create interesting, new topnotes.

This aldehyde finds even more use in flavor compositions, particularly in Strawberry, Banana, Apple, Apricot, Plum, Pear and many berry or fruit complexes. In Orange flavors it may introduce a much wanted "lift" to the freshness of such sweet flavor.

Concentrations are low, about 0.7 to 20 ppm in the finished product.

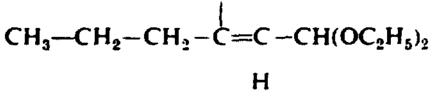
A special use is in Cucumber imitation flavor, also occasionally asked for in perfumes for hand-lotions, etc. It forms an important part of the natural aldehyde portion in the aroma of Cucumber.

G.R.A.S. F.E.M.A. No.2560.

Prod.:
1) by reduction of Hexenoic acid with Formic acid vapors over Manganese dioxide at 350° C.
2) by oxidation of the corresponding Hexenol.
3) by condensation of Acetaldehyde with *n*-Butyraldehyde.

89-38; 158-149; 158-252; 156-25; 140-159;

## 1600: trans-2-HEXENAL DIETHYLACETAL



$$CH_3-CH_2-CH_2-\overset{H}{C}=\underset{H}{C}-CH(OC_2H_5)_2$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Fruity-green, refreshing and rather mild odor, reminiscent of Appleskins or unripe Apples.

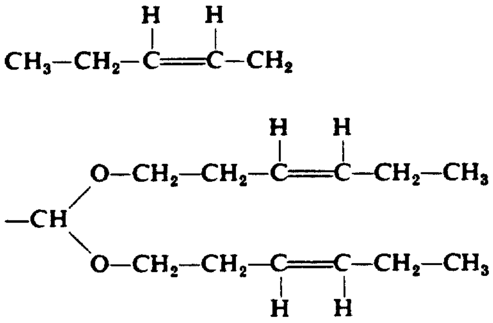
Suggested for use in perfume compositions, this acetal should not be considered as a variation of the aldehyde. It has its own odor and character, and since it is much milder, it is easier to apply to experimental perfumes. The greenness is not sharp and not typically leafy. It has a caramellic undertone resembling that found in Citral diethylacetal and other acetals.

Once approved by the authorities for use in food flavors, this acetal could find use in various compositions, such as imitation Gooseberry, Apple, Wine, Grape, etc.

Prod.: from *trans-2*-Hexenal and Ethanol by condensation.

(Sample: Compagnie Parento, Inc.).

## 1601: cis-3-HEXENAL-DI-cis-3-HEXENYL ACETAL



$C_{18}H_{32}O_2 = 280.45$

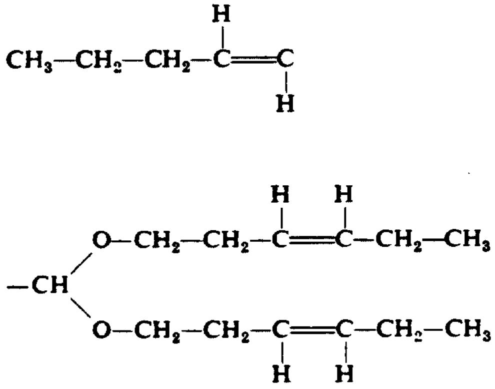
Colorless liquid. Insoluble in water (decomposes slowly), soluble in alcohol and oils.

This Acetal – like the isomer described in the following monograph, is, in the author's opinion, of no more than academic interest. Beyond mention of its mere existence on a research shelf, the literature brings no facts about the material.

Its apparent instability in aqueous media should also warn against the belief that one could get entirely novel aromas out of such Acetals, the components of which are already known and widely used.

Prod.: by condensation of *cis-3*-Hexenal with *cis-3*-Hexenol, using a catalyst and dehydrating agent. The reaction is susceptible to produce a number of by-products.

## 1602: trans-2-HEXENAL-DI-cis-3-HEXENYL ACETAL



$C_{18}H_{32}O_2 = 280.45$

Colorless liquid. Insoluble in water (decomposes slowly), soluble in alcohol and oils.

This Acetal has been produced – as one could expect – in the hope to find a very natural green odor in combining the forces and virtues of Leaf alcohol with the so-called "Leaf aldehyde" (see also the previous monograph on the Acetal of *cis-3*-Hexenal).

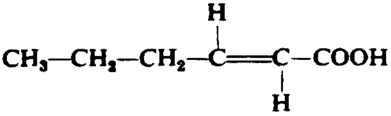
Apparently never in commercial production, this material has not (yet) aroused sufficient interest to warrant its regular production.

Literature on the subject contains no facts. and the author believes that this Acetal has only academic interest.

89-40;

## **1603:** trans-2-**HEXENOIC ACID**

Hexen-*2*-oic acid.
*beta*-Propyl acrylic acid.
*alpha-beta*-Hexenoic acid.
*alpha-beta*-Hexylenic acid.



$CH_3{-}CH_2{-}CH_2{-}\overset{H}{C}{=}\underset{H}{C}{-}COOH$

$C_6H_{10}O_2 = 114.15$

Colorless, needle-like crystals. M.P. 37° C. B.P. 217° C. Sp.Gr. 0.97 (liquid).

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Fatty and slightly acrid-musty odor in the pure state, pleasant, fruity-sweet odor in dilution. Powerful and comparatively tenacious.

In dilutions below 50 ppm, the flavor is pleasant, fruity-warm, somewhat herbaceous, discretely acid. In higher concentration it shows pungency and less pleasant, acid notes.

This acid, only recently commercially available, is mainly used in flavor compositions. Its most interesting place is in imitation Raspberry, but it can find its place in many other fruit flavors where the caramellic-acid note lends richness and naturalness to an otherwise chemical Aroma.

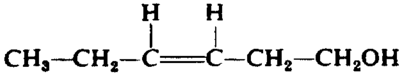
It is rarely used in perfumes, except occasionally in the reconstruction of essential oils, etc.

Prod.: by condensation of Butyraldehyde with Malonic acid.

66-637; 90-121; 160-1036;
(sample: Compagnie Parento, Inc.).

## **1604:** cis-3-**HEXENOL**

*beta-gamma*-Hexenol.
*n-beta*-Hexenol.
*primary-n*-Hexylenic alcohol (old name).
"Phyllol" (Schimmel).
"Verdalol" (Schimmel).
"Leaf alcohol" (this name also used for *trans-2*-Hexenol).



$CH_3{-}CH_2{-}\overset{H}{C}{=}\overset{H}{C}{-}CH_2{-}CH_2OH$

$C_6H_{12}O = 100.16$

Colorless liquid. B.P. 157° C. Sp.Gr. 0.86.

Slightly soluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful and intensely green, grassy odor. It appears more grassy-green and foliage-green, less fruity than the *trans-2*-Hexenol.

Although quite frequently used in perfume compositions, this alcohol remains a "small item" with respect to volume. It is an extremely powerful odorant, and its application in perfumery is somewhat limited to certain types of topnote formulations. It is also used in the construction of artificial essential oils and flower absolutes, but the availability of *trans-2*-Hexenol reduces the interest in the subject isomer to a considerable degree.

Traces of *cis-3*-Hexenol are used in refreshing topnotes in delicate floral fragrance types, such as Muguet and Lilac, and the alcohol is often used along with Geranium oil, Galbanum, Oakmoss, Lavender and Mint oils in various fragrance types.

In flavors, this alcohol find its way into imitation Mint and in various fruit complexes, always in mere traces. The concentration used is about 1 to 5 ppm in the finished product.

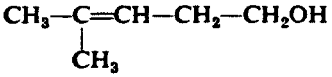
G.R.A.S. F.E.M.A. No.2563.

Prod.: from Tetrahydro furan. A number of patented methods are well guarded by the numerous producers of this alcohol. Several methods include selective hydrogenation of Hex-*3*-yne-*1*-ol.

2-716; 4-61; 34-1210; 86-58; 87-479; 156-17; 140-125;

## 1605: iso-HEXENOL

*4*-Methyl-*3*-penten-*1*-ol.
Sometimes commercially called:
*iso-beta-gamma*-Hexenol.



$$CH_3-\underset{\substack{|\\ CH_3}}{C}=CH-CH_2-CH_2OH$$

$C_6H_{12}O = 100.16$

Colorless mobile liquid.

Very slightly soluble in water, soluble in alcohol and oils.

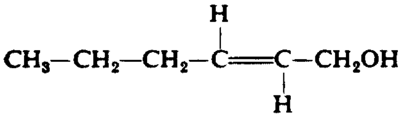
Powerful, gassy-green, but rather sharp odor, even in dilution not closely reminiscent of any natural green odor.

This olefinic alcohol has found a little use in perfumery, but the author is of the impression that it has been outperformed by its much more popular isomers – at least as far as natural green notes are concerned.

Prod.: (several methods) e. g. from *beta-iso*-Amylenyl Magnesium bromide plus Trioxymethylene by Grignard type reaction.

## 1606: trans-2-HEXENOL

*gamma*-Propyl allyl alcohol.
*2*-Hexenol.
"Leaf alcohol" (sometimes called). This name is also used for *cis-3*-Hexenol.



$$CH_3-CH_2-CH_2-\overset{\substack{H\\ |}}{C}=\underset{\substack{|\\ H}}{C}-CH_2OH$$

$C_6H_{12}O = 100.16$

Colorless liquid. Sp.Gr. 0.85. B.P. 155° C.

Very slightly soluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful, fruity-green, slightly caramellic-fruity in its undertone and with an overall odor often compared to that of Chrystanthemum foliage, or wine leaves. The odor is sweeter, more winey-leafy than that of the *cis-3*-Hexenol.

Although quite interesting in perfume formulations, this alcohol finds its greatest field in flavors. Its taste is sweeter, more fruity than that of the *cis-3*-Hexenol.

Its use in perfumes is somewhat limited. Lavender and Lavandin oil compositions may benefit from the topnote created with this alcohol, and certain floral bouquets can be improved with pleasantly green, sweet and natural notes from the subject material. It finds increasing use in artificial Geranium oils.

In flavors, traces are used in fruit complexes, and it is a common ingredient in artificial Strawberry. It adds freshness to Mint compositions, and it is often used to reconstitute the flavor in Orange juice, whose flavor suffers severely during the processing.

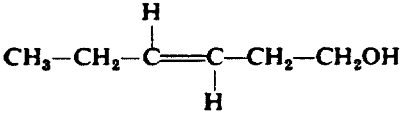
G.R.A.S. F.E.M.A. No.2562.

Prod.: from Propyl vinyl carbinol by heating with Aluminium oxide. A number of other methods are well-guarded secrets of many producers of this alcohol.

87-479; 156-17; 140-125;
see also: Journal of Food Science, 29, 790 (1964).
(Samples: Fritzsche Bros. Co., Inc. and Compagnie Parento, Inc.).

## 1607: trans-3-HEXENOL

Formerly called: "*iso-beta-gamma*-Hexenol".



$$CH_3-CH_2-\overset{\substack{H\\ |}}{C}=\underset{\substack{|\\ H}}{C}-CH_2-CH_2OH$$

$C_6H_{12}O = 100.16$

Colorless liquid. Sp.Gr. 0.86. B.P. 165° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Intensely green, but rather "bitter"-foliage-like, somewhat fatty odor. More "Chrysanthemum-like" and less fruity than its two isomers.

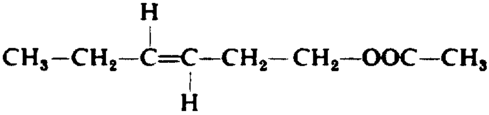
This alcohol finds a little use in perfumery as part of "green" topnote compositions, as a modifier for its isomers, and in herbaceous fragrances, Fougères, etc. to introduce new nuances of natural foliage odors. It is not nearly as versatile as *trans-2*-Hexenol, and not as generally pleasant smelling as *cis-3*-Hexenol.

Prod.: Among many processes, it often appears as a by-product in the manufacture of its isomers.

156-17;

## 1608: cis-3-HEXENYL ACETATE

*cis-beta-gamma*-Hexenyl acetate.
"Verdural extra" (I.F. & F.).
- and many other trade names.



$CH_3-CH_2-\overset{H}{C}=\underset{H}{C}-CH_2-CH_2-OOC-CH_3$

$C_8H_{14}O_2 = 142.20$

Colorless mobile liquid. Sp.Gr. 0.91.
B.P. 169° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Intensely green, sharp-fruity and very diffusive odor, in dilution reminiscent of unripe Banana peel.

In dilutions below 10 ppm it produces very pleasant fruity-green flavors, and its taste individually at concentrations below 2 ppm is distinctly Banana-like.

Very interesting combination flavors can be created with this ester and a few other chemicals: A concentration of about 1 ppm of *cis-3*-Hexenyl acetate in the presence of 0.05 ppm Allyl-*iso*-thiocyanate (Allyl mustard oil) will produce a distinct note of unripe Banana with the sharp greenness and the fruity notes unmistakably identifiable as Banana and absolutely no impression of Mustard. The two materials separately at the concentrations indicated give very weak and incomplete flavor pictures.

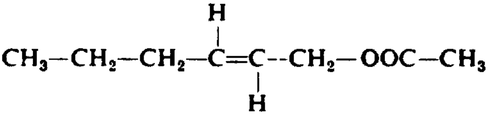
However, this ester finds considerable use in perfumes, where it may lend pleasant and natural freshness to delicate florals (Muguet, Lilac, Narcisse, etc.) and participate in creating true-to-Nature, foliage-green topnotes in other fragrance types. The ester is most likely to supersede the less stable and less natural smelling Alkyl acetylenic esters, slowly being abandoned in modern perfumery.

Prod.: by esterification of *cis-3*-Hexenol with Acetic acid under azeotropic conditions.

2-717; 4-61; 156-17;

## 1609: trans-2-HEXENYL ACETATE

2-Hexenyl acetate.



$CH_3-CH_2-CH_2-\overset{H}{C}=\underset{H}{C}--CH_2-OOC-CH_3$

$C_8H_{14}O_2 = 142.20$

Colorless liquid. Sp.Gr. 0.91. B.P. 166° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and fresh-green, sweet and fruity, very "natural" odor.

Powerful, fresh-fruity, Banana-like, Apple- and Pear-like, somewhat green, but overall sweet taste in dilutions below 2 ppm.

This ester is primarily used in flavor compositions, since it is more fruity than the *cis-3*-Hexenyl acetate, and less sharp-green. Among the few places in perfumery where it may find good use are certain artificial essential oils such as Geranium, Clary Sage, Ylang-Ylang, etc.

The ester is used in various fruit imitation flavors in minute traces, so that the concentration in the finished products is rarely more than 0.3 to 2 ppm. Banana, Apple, Pear, Melon, etc. are among the many types where this ester can be useful.

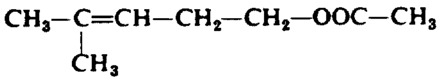
Prod.: by esterification of *trans-2*-Hexenol with Acetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2564.

156-17; 90-221;
(sample: Compagnie Parento, Inc.).

## 1610: iso-HEXENYL ACETATE

*4*-Methyl-*3*-penten-*1*-yl acetate.
Sometimes called *iso-beta-gamma*-Hexenyl acetate.



$$CH_3-\underset{CH_3}{\underset{|}{C}}=CH-CH_2-CH_2-OOC-CH_3$$

$C_8H_{14}O_2 = 142.20$

Colorless liquid.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Penetrating, gassy-green diffusive odor of poor tenacity. There are fruity undertones, but they appear only in proper dilution, when the pungent gassy green notes are subdued.

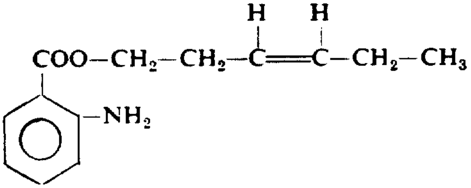
This ester has been available and was suggested for use in perfume compositions before the time when the *2*- and *3*-Hexenyl esters became readily available at attractive cost.

The title ester is probably the least "natural" of the known isomers of this series, and it will most likely become obsolete in perfumery.

The author sees no future for this ester in flavor creation.

Prod.: by azeotropic type esterification of the alcohol (see monograph).

## 1611: cis-3-HEXENYL ANTHRANILATE



$C_{13}H_{17}NO_2 = 219.29$

Pale straw-colored or pale amber-colored, somewhat viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Darkens upon exposure to daylight.

Very sweet and tenacious, fruity, American Concord-Grape-like odor.

Sweet, fruity-floral taste with distinctly Grape-and-wine-like note.

The odor type of this ester limits its use to a very few possible applications in perfumery, perhaps as a modifier in Colognes, Neroli bases, Petitgrain compositions, etc.

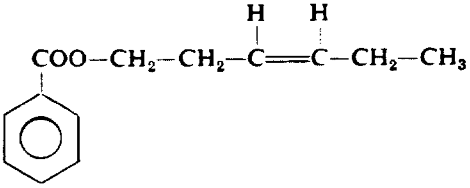
The ester is not specifically listed in the American Federal Register as G.R.A.S., and its use in food flavors is therefore not permitted in the U.S.A.

In view of the fact that this material was probably developed in search of interesting esters of the Hexenols, and not in the intention of producing an already existing natural chemical, there is little chance of future need or use of this ester.

Prod.: by esterification of *cis-3*-Hexenol with Anthranilic acid, which can alternatively be undertaken as a cross-esterification or a trans-esterification with Methyl anthranilate as one component.

(Sample: Compagnie Parento, Inc., 1966).

## 1612: cis-3-HEXENYL BENZOATE



$C_{13}H_{16}O_2 = 204.27$

Colorless, slightly viscous liquid.
Sp.Gr. 1.01. B.P. 256° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, but tenacious, green-herbaceous and woody odor.

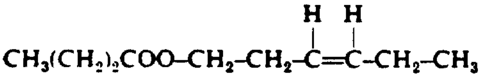
The major asset of this ester is its tenacity. As a "green" material it is much weaker than the esters of the lower alifatic acids. But the milder odor makes it easier to handle, and the gentle, green-herbaceous effect can be suitably utilized in Fougeres, New Mown Hay compositions, Chypres, etc. It blends very well with Styrax materials and the Phenylethyl alcohol family, with Amyl salicylate and Coumarin, Oakmoss and Ylang-Ylang.

Prod.: by esterification of *cis-3*-Hexenol with Benzoic acid (or with Benzoyl chloride).

156-17;
(sample: Compagnie Parento, Inc. 1966).

## 1613: cis-3-**HEXENYL BUTYRATE**

*beta-gamma*-Hexenyl-*n*-butyrate.



$$CH_3(CH_2)_2COO-CH_2-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_3$$

$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. Sp.Gr. 0.90. B.P. 192° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful, fruity-winey, green, Cognac-like or Brandy-like, slightly buttery-oily odor.

Winey-buttery, sweet-green and slightly fruity taste in dilutions below 5 ppm.

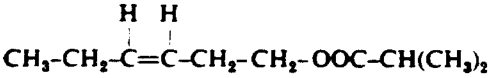
This ester has been suggested for use in perfume compositions as a modifier for the Acetate and other esters. As a green topnote material, it blends better with certain floral fragrance types, e. g. Jasmin and Ylang-Ylang, while it also gives interesting effects with strictly herbaceous odor types, where winey-green notes can support Clary Sage or other sweet-herbaceous, ot tea-like notes.

Prod.: by esterification of *cis-3*-Hexenol with *n*-Butyric acid under azeotropic conditions.

156-17;
(sample: Compagnie Parento, Inc. 1966).

## 1614: cis-3-**HEXENYL**-iso-**BUTYRATE**

*beta-gamma*-Hexenyl-*iso*-butanoate.



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-OOC-CH(CH_3)_2$$

$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. Sp.Gr. 0.89. B.P. 182° C.

Practically insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

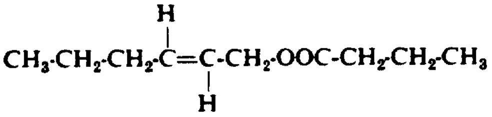
Fruity-winey, sweet-green odor of considerable power and diffusion. Powerful and sweet, Apple-like taste.

As compared to the *n*-Butyrate, this ester is less buttery, more fruity in its overall odor type. It is perhaps less reminiscent of natural products except Apple, and has therefore not become very popular. It could find use as a modifier for the Hexenyl esters with lower acids, and it will blend particularly well with fruity notes of the Apple-Peach-Apricot type (Undecanolide, etc.). It lends freshness to Lavender and other herbaceous fragrances, and gives lift to many types of floral fragrance.

Prod.: by esterification of *cis-3*-Hexenol with *iso*-Butyric acid under azeotropic conditions.

## 1615: trans-2-HEXENYL BUTYRATE

2-Hexenyl-*n*-butyrate.



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{H}{C}{=}\underset{H}{C}\text{-}CH_2\text{-}OOC\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

$C_{10}H_{18}O_2 = 170.25$

Colorless liquid. Sp.Gr. 0.88. B.P. 190° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, fruity-green, herbaceous-sweet and somewhat winey odor of moderate tenacity.

Sweet, green-fruity, winey and slightly buttery taste.

This ester, not a very commonly used member of the series, could find some use in perfume compositions and artificial essential oils. It is most conceivable, however, that the material will find more interest in the flavor laboratory.

As a trace in component various fruit compositions, it could lend interesting and natural notes to Apricot, Apple, Pineapple, Plum and to various Cognac or Brandy flavor compositions.

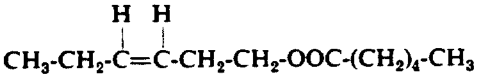
The concentration used would normally be about 0.5 to 2 ppm calculated upon the finished product.

Prod.: by esterification of *trans-2*-Hexenol with *n*-Butyric acid under azeotropic conditions.

156-17; 90-221;
(sample: Compagnie Parento, Inc.).

## 1616: cis-3-HEXENYL CAPROATE

*beta-gamma*-Hexenyl hexoate.



$$CH_3\text{-}CH_2\text{-}\overset{H}{C}{=}\overset{H}{C}\text{-}CH_2\text{-}CH_2\text{-}OOC\text{-}(CH_2)_4\text{-}CH_3$$

$C_{12}H_{22}O_2 = 198.31$

Colorless liquid.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful fruity-green, diffusive odor, more fruity, less green than the Acetate or the Butyrate. Is is also somewhat sharper than the *trans-2*-Hexenyl caproate (see next).

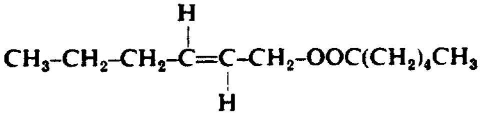
This ester has been suggested for use in perfumes and flavors. The author believes that it will primarily find application in flavors, where its Pear-Pineapple character and comparatively powerful Aroma could blend with the conventional materials in such flavor compositions.

As a novel note in modern fragrances, it could form part of fruity-green topnote complexes, a type which is rather popular lately.

Prod.: by esterification of *cis-3*-Hexenol with *n*-Hexanoic acid under azeotropic conditions.

## 1617: trans-2-HEXENYL CAPROATE

2-Hexenyl-*n*-hexanoate.



$$CH_3\text{–}CH_2\text{–}CH_2\text{–}\overset{H}{C}{=}\underset{H}{C}\text{–}CH_2\text{–}OOC(CH_2)_4CH_3$$

$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Sp.Gr. 0.89. B.P. 220° C.

Practically insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful, fruity, sweet and diffusive odor, reminiscent of Apple, Pear and Pineapple.

Sweet-fruity, Apple-like taste, reminiscent of the skin of Reinette Apples, also of Pear. Pleasant concentration level is about 5 ppm.

This ester is suggested for use in flavor compositions, mainly imitation Apple, Pear, Pineapple, etc. but also in the popular "Tutti-frutti" types, where its radiance and power produces highly desirable effects.

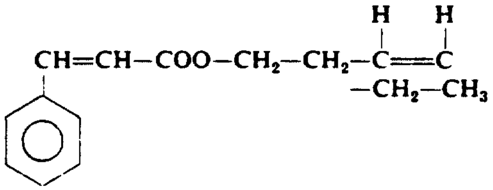
It can also be used in perfume compositions, although for this purpose, it is perhaps less suitable than the *cis-3*-isomer (see previous monograph). The subject ester is sweeter and less green than the *cis-3*-Hexenyl caproate. It may act as an interesting modifier for Galbanum and other "green" naturals in various modern fragrance compositions and their top-note complexes.

Prod.: by esterification of *trans-2*-Hexenol with *n*-Hexanoic acid under azeotropic conditions.

156-17;
(sample: Compagnie Parento, Inc.).

## 1618: cis-3-HEXENYL CINNAMATE

*beta-gamma*-Hexenyl phenylacrylate.



$C_{15}H_{18}O_2 = 230.31$

Colorless or pale straw-colored, viscous liquid.
B.P. 293° C. Sp.Gr. 1.01.

Practically insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

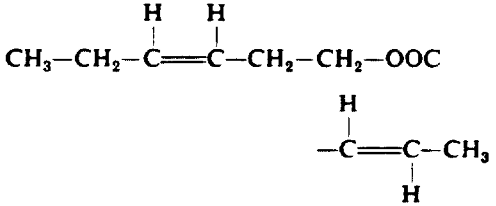
Mild balsamic-green, somewhat herbaceous and refreshing odor of considerable tenacity.

This ester, a member of a very long series of Hexenyl esters, is not among the most interesting ones. The author finds, that it may have only little more than academic interest, since it does not offer any unusual notes or effects other than those obtainable with several other members of the Hexenyl family plus suitable Cinnamic derivatives.

156-17;
(sample: Compagnie Parento, Inc., 1966).

## 1619: cis-3-HEXENYL CROTONATE

*beta-gamma*-Hexenyl-*trans-2*-butenoate.



$CH_3{-}CH_2{-}\overset{H}{C}{=}\overset{H}{C}{-}CH_2{-}CH_2{-}OOC{-}\overset{H}{C}{=}\underset{H}{C}{-}CH_3$

$C_{10}H_{16}O_2 = 168.24$

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Powerful, dry-green odor with floral undertones.

This ester, produced by very few perfume chemical manufacturers only, has been suggested for use in floral fragrances as a natural-green topnote item.

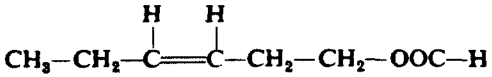
It blends very well with Galbanum and with the "carbinols" conventionally used in Hyacinth or Lilac bases, and its greenness is pleasantly different from the penetratingly diffusive odor of some of the lower esters of the Hexenyl series. Its peculiar dry note seems to rule out any predominant fruity tone which is so common in many of these esters.

Prod.: by direct esterification of *cis-3*-Hexenol with Crotonic acid.

(Sample: Norda Ess. Oil & Chem. Co., Inc.).

## 1620: cis-3-HEXENYL FORMATE

*beta-gamma*-Hexenyl methanoate.



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-OOC-H$$

$C_7H_{12}O_2 = 128.17$

Colorless liquid. Sp.Gr. 0.92. B.P. 155° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Dry-green, petal-like and vegetable-like odor with waxy-sweet undertones. The "vegetable" notes resemble those of Cucumber and Radish, yet without the sharpness of the latter. To some observers, it also appears floral.

Semi-sweet, fresh-vegetable-green taste in dilutions below 2 ppm.

This ester finds some use in perfumery as part of various topnote complexes. It blends very well with Galbanum and with many herbaceous oils. Styrax is a good fixative, and supporting fixation and blending can be achieved with Cinnamates. The ester could constitute the main part of the green theme in Hyacinth when suitably incorporated.

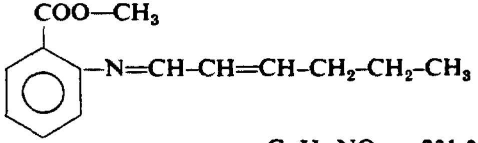
In flavors, it forms an excellent combination with Nonadienal and Nonadienol in Cucumber compositions and other vegetable, juicy-green flavor types. It is furthermore a generally refreshing modifier for the higher esters of the series.

Prod.: from *cis-3*-Hexenol and Formic acid, e. g. in presence of Acetic anhydride in cold Formylation.

156-17;

## 1621: HEXENYLIDENE METHYLANTHRANILATE

A "Schiff's base" type condensation product.



$C_{14}H_{17}NO_2 = 231.30$

Yellowish oily or viscous liquid, occasionally with a greenish tint. Insoluble in water, soluble in alcohol and oils.

Powerful and very sweet, but refreshingly citrusy, floral odor of good tenacity. Variations in method of production (different manufacturers) result in considerable difference in odor characteristics. Traces of surplus aldehyde will completely override the true odor of the condensation product, while surplus of the Methylanthranilate causes a dull, musty odor in the picture.

This "base" finds use in perfume compositions mainly as a fixative in the lighter portion of modern Citrus-type colognes (which are, to be correct, revived old-fashioned types).

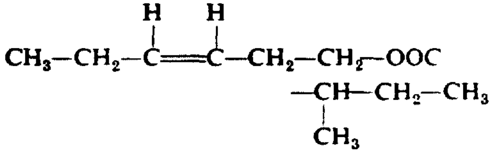
The material is rarely found in price lists under its proper chemical name, but it is mostly sold in the shape of bases in which it may be only a minor ingredient (with respect to volume).

It blends very well with Petitgrain oil, Neroli, Grapefruit and Bitter Orange oils, Lemon and Lime oils, with the alifatic aldehydes and Lilial (Bucinal) or Cyclamal, etc. but it will rarely exceed a few percent of the final composition.

Prod.: from *trans-2*-Hexenal and Methylanthranilate by condensation usually at not less than 65° C. for 3 to 6 hours under mild vacuum to remove water quantitatively.

## 1622: cis-3-HEXENYL-alpha-METHYL BUTYRATE

*cis-3*-Hexenyl-*2*-methylbutanoate.



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-OOC-\underset{CH_3}{CH}-CH_2-CH_3$$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Rich and powerful, warm-fruity odor of a distinctly "unripe" Apple-Pineapple character and pleasant overall freshness.

Sweet-herbaceous-fruity Apple-like taste in dilutions below 5 ppm.

In spite of the "unripe" odor in high concentration, this ester produces very "ripe" fruity notes in dilutions and combinations with suitable blenders. It has good tenacity.

It finds use in perfume compositions and artificial essential oils as a "naturalizer" and freshener-modifier for the more green notes of lower esters of Hexenol. It blends particularly well with Lavender, Lavandin, Clary Sage and Geranium.

In flavors, it offers good opportunities for variation of the Apple and Pine-apple themes with conventional materials. In Plum, Peach and Apricot, where overly sweet fruity notes may be prevalent, it will supply sufficient freshness to compensate for those heavy Aromas of other chemicals.

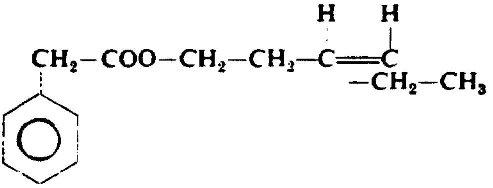
Esters of *alpha*-Methylbutyric acid have become quite popular since more and more such esters have been identified in natural products. Approved for use in food flavors by the American F. R. 1965.

Prod.: from *cis-3*-Hexenol by esterification with *alpha*-Methylbutyric acid under azeotropic conditions.

(Sample: Compagnie Parento, Inc.).

## 1623: cis-3-HEXENYL PHENYLACETATE

*beta-gamma*-Hexenyl-*alpha*-toluate.



$C_{14}H_{18}O_2 = 218.30$

Colorless, slightly viscous liquid.
Sp.Gr. 1.00. B.P. 299° C.

Insoluble in water, soluble in alcohol and oils.

Mild and sweet, green-rosy-mossy odor with undertones of herbaceous-woody, somewhat condiment-vegetable-like character.

Some observers report that they find Onion-like or spicy notes in the odor of this ester.

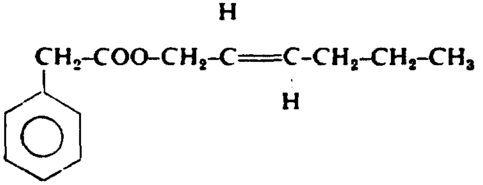
Recommended for Mint flavor compositions, this ester has probably very limited application. The fact that it is a component of Mentha arvensis oil, does not increase the interest in such material very much. Mentha arvensis oil, the least expensive of all the Mint oils, should be in no danger of being "artificially reconstructed", and the subject ester does not seem to be a key ingredient in the oil.

As a trace component in certain flavor compositions, this ester might well find some use. It is, however, not yet listed as G.R.A.S. in the American Federal Register.

Prod.: from Phenylacetyl chloride and *cis-3*-Hexenol with Pyridine catalyst in an inert diluent.

90-342; 156-17;

## 1624: trans-2-HEXENYL PHENYLACETATE



$C_{14}H_{18}O_2 = 218.30$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Green-mossy, very tenacious odor with variable amounts of the almost unavoidable honey-like notes (presumably from excess Phenylacetic acid), but an overall character that leaves the observer with the question: where can I possibly use this chemical?

It may be somewhat typical of the rare Phenylacetates that they do not lend themselves very obviously to an application, and they are – on the other hand – very sensitive to variations in method of production, ratio of acid/alcohol/ester in the finished chemical, etc.

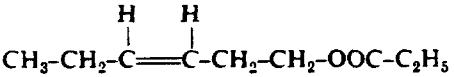
The author has the impression that this chemical may be one of the less interesting esters of the Hexenyl series, and the fact that its isomer has been found in measurable quantity in certain Mint oils is not sufficient to encourage wider usage of it.

Prod.: from *trans-2*-Hexenol and Phenylacetic acid under azeotropic esterification conditions.

(Sample: Fritzsche Bros. Inc.).

## 1625: cis-3-HEXENYL PROPIONATE

*beta-gamma*-Hexenyl propanoate.



$CH_3\text{-}CH_2\text{-}\overset{H}{C}{=}\overset{H}{C}\text{-}CH_2\text{-}CH_2\text{-}OOC\text{-}C_2H_5$

$C_9H_{16}O_2 = 156.23$

Colorless liquid. Sp.Gr. 0.91. B.P. 172° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Sweet, powerful, intensely green, somewhat "vegetable"-like but also slightly fatty, oily odor.

The taste is not purely sweet or fruity, and it is pleasant only at very low level (below 2 ppm).

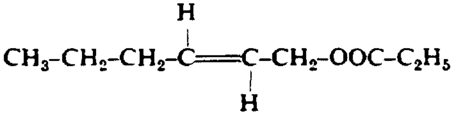
Suggested for use in perfume compositions, mainly as a modifier for the Acetate, which tends to be overly fruity. However, since the Propionate does not resemble any particular natural material, it seems to be less popular than most of the other esters.

Prod.: from *cis-3*-Hexenol and Propionic acid by azeotropic esterification.

156-17;
(sample: Compagnie Parento, Inc. 1966).

## 1626: trans-2-HEXENYL PROPIONATE

2-Hexenyl propanoate.



$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{H}{C}{=}\underset{H}{C}\text{-}CH_2\text{-}OOC\text{-}C_2H_5$

$C_9H_{16}O_2 = 156.23$

Colorless liquid. Sp.Gr. 0.87. B.P. 169° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful and diffusive, fruity-sweet odor, free from fatty notes. More fruity, more sweet than the *cis*-isomer, and not so dry in its greenness.

The taste is powerfully fruity, somewhat green, but sweet in dilutions below 5 ppm.

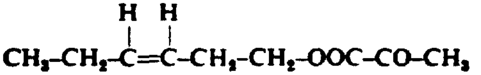
This ester lends itself more to flavor compositions than to perfumes. It could be used in Tutti-frutti-compositions as a powerful factor, or as a modifier in Apple, Pear, Pineapple or Peach, but it is not quite as versatile as the Acetate or the Butyrates.

Prod.: by esterification of *trans-2*-Hexenol with Propionic acid under azeotropic conditions.

156-17;
(sample: Compagnie Parento, Inc., 1966).

## 1627: cis-3-HEXEN-1-YL PYRUVATE

*cis-3*-Hexen-*1*-yl-*2*-oxopropanoate.
Hexenyl pyruvate.



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-OOC-CO-CH_3$$

$C_8H_{14}O_3$ = 170.21

Colorless or pale straw-colored liquid.

Sweet, spicy-caramellic, relatively mild odor of moderate tenacity. The green notes are practically concealed in a warm-aromatic, almost spicy fragrance.

Sweet, somewhat spicy-caramellic taste in dilutions below 20 ppm. Pungent, slightly burning at higher concentrations.

This ester finds use almost exclusively in flavor compositions. Its particular aroma does not lend very attractive notes to a perfume composition.

The main use is that of being a major modifying component of imitation (or reconstructed) Celery flavor, the chief components of which are two or more members of the Butylidene dihydrophthalide family.

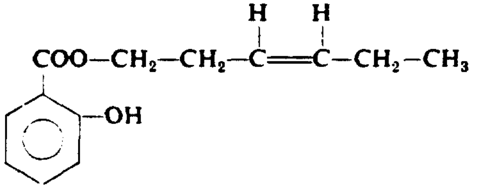
Normal concentration will be of the order of magnitude of approximately one-tenth of the amount of Dihydrophthalide-derivatives used.

Prod.: by esterification of *cis-3*-Hexenol with Pyruvic acid under azeotropic conditions.

158-146;
see also: Dr. H.J.Gold: Journal of Food Science 28, 484 (1963). (Also presented at the American Chemical Society meeting and Food Flavor Symposium, Detroit, Mich. April 1965).
(Sample: Compagnie Parento, Inc.).

## 1628: cis-3-HEXENYL SALICYLATE

*beta-gamma*-Hexenyl salicylate.



$C_{13}H_{16}O_3$ = 220.27

Colorless oily liquid. Sp.Gr. 1.06.
B.P. 271° C.

Insoluble in water, soluble in alcohol and oils.

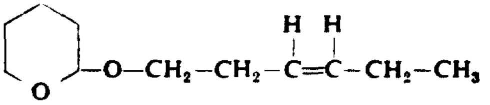
Sweet, slightly green-balsamic, tenacious odor. More green and less floral than Hexyl salicylate.

The author is of the impression that this ester is not one of the more interesting ones of the Hexenyl series. It has only moderate power and its green plus sweet notes do not produce any very unusual or particularly desirable effect in perfumes. It is most likely that this ester will become obsolete in the near future.

Prod.: from *cis-3*-Hexenol and Salicylic acid by azeotropic type esterification.

156-17;
(sample: Compagnie Parento, Inc., 1966).

## 1629: cis-3-HEXENYL-TETRAHYDRO-2-PYRANYLETHER



$C_{11}H_{20}O_2$ = 184.28

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very powerful, in concentrated form "gassy"-green, but sweet and rich, in extremely diluted form more floral-sweet with a natural leafy note. It is most conceivable that the few samples shown to the author have been chemically impure, possibly mixtures of isomers and homologues of the title chemical.

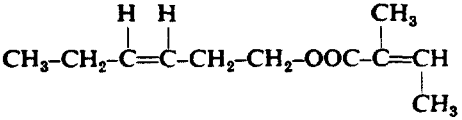
This ether has been introduced into the perfumery world as a new power component in the imitation of natural notes for Rose and "greenness" along with floral power. Its beauty and usefulness is only understood and appreciated when the material is brought to proper dilution, which in most cases will be near one percent of the finished perfume composition. Concentrations of 0.1% are often effective and pleasantly perceptible, while concentrations above 1% may require special creative effort to build a suitable "frame" around the powerful chemical. It forms excellent combination odors with Rose oxide, but the two chemicals both suffer from the fact that they are rarely offered in the pure form, i. e. as one single, well-defined chemical. Work with these materials should therefore still be considered experimental, but it is extremely challenging and promising.

The title ether is a higher homologue of Rose oxide (remotely related) besides of being a Pyranyl ether, where Rose oxide is a Pyran derivative.

Prod.: e. g. from *2:3*-Dihydro-*gamma*-pyran with *cis-3*-Hexenol.

## **1630:** cis-3-**HEXENYL TIGLATE**

*cis-3*-Hexenyl-*2*-methyl-*trans-2*-butenoate.



$CH_3\text{–}CH_2\text{–}\overset{H}{C}=\overset{H}{C}\text{–}CH_2\text{–}CH_2\text{–}OOC\text{–}\overset{CH_3}{C}=\underset{CH_3}{CH}$

$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Fresh, powerful, yet relatively tenacious deep-green foliage odor with slightly fruity-fatty undertones.

This ester finds a little use in the reconstruction of various essential oils, and as part of the topnote complex in modern, green-herbaceous fragrances and as a fresh topnote element in florals and bouquets.

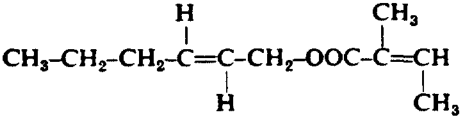
Its aroma differs substantially from that of the saturated ester, which is not at all green, but very warm-herbaceous and winey, resembling notes in Roman Chamomile oil. It is therefore doubtful if the subject ester will find much use in flavor compositions, except as a trace component modifier in certain fruit and vegetable flavor compositions.

Prod.: from *cis-3*-Hexenol and Tiglic acid by direct esterification.

(Sample: Compagnie Parento, Inc., 1966).

## **1631:** trans-2-**HEXENYL TIGLATE**

*trans-2*-Hexenyl-*2*-methyl-*trans-2*-butenoate.



$CH_3\text{–}CH_2\text{–}CH_2\text{–}\overset{H}{C}=\underset{H}{C}\text{–}CH_2\text{–}OOC\text{–}\overset{CH_3}{C}=\underset{CH_3}{CH}$

$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, green and sweet odor with a fruity undertone and moderate tenacity.

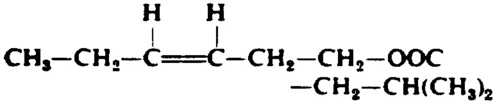
Warm and somewhat herbaceous taste, not purely sweet, but slightly fruity and relatively powerful. Pleasant level: below 5 ppm.

This isomer is very rarely offered commercially, but it has been suggested for use in perfumes and flavors. The author finds that it would most likely find more use in flavors than in perfumes. This material could be used as a modifier in various Berry type flavors: Strawberry, Blackcurrant, Gooseberry, etc. but the effect is, as above mentioned, not purely sweet or fruity.

Prod.: by esterification of *trans-2*-Hexenol with Tiglic acid.

## 1632: cis-3-HEXENYL-iso-VALERATE

*beta-gamma*-Hexenyl-*iso*-pentanoate.



$$CH_3-CH_2-\overset{H}{C}=\overset{H}{C}-CH_2-CH_2-OOC-CH_2-CH(CH_3)_2$$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Sp.Gr. 0.89. B.P. 199° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Relatively powerful, sweet-green, Apple-like odor with buttery-creamy notes.

Powerful, green-fruity, buttery and sweet taste, reminiscent of Apples. Pleasant concentration level: less than 5 ppm.

This ester finds some use in flavor compositions as a power ingredient and modifier in Apple, Pear, Pineapple, Plum, etc. where it helps introduce natural freshness in balance with possible overly sweet notes from conventional flavor chemicals.

As a novel type modifier in Peppermint flavors, it should have good possibilities in the future.

The author knows of no important use of this ester in perfume compositions.

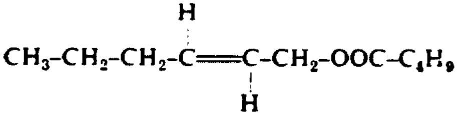
Approved for use in food flavors by the American F.R. 1965.

Prod.: by direct esterification of *cis-3*-Hexenol with *iso*-Valeric acid under azeotropic conditions.

156-17;
(sample: Compagnie Parento, Inc., 1966).
NOTE: The stereo-isomer *trans-2*-Hexenyl-*iso*-valerate and its isomer, the *n*-Valerate, have both been commercially produced, and it is possibly too early to say which isomer will become most popular (see next).

## 1633: trans-2-HEXENYL VALERATE

NOTE: Commercial production of the *iso*-Valerate seems to have been discontinued, while the *n*-Valerate is occasionally produced since 1967.



$$CH_3-CH_2-CH_2-\overset{H}{C}=\underset{H}{C}-CH_2-OOC-C_4H_9$$

$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Almost insoluble in water, soluble in alcohol, Propylene glycol and oils, but poorly soluble in Glycerin. Sp.Gr. 0.87.

Powerful and diffusive, sweet, buttery-creamy and fruity-winey odor. It appears less Apple-like than the odor of the *cis-3*-Hexenyl *iso*-valerate (see previous monograph) and much more creamy at suitable dilution (approximately 5 ppm or lower).

This ester – particularly the *trans-2*-Hexenyl-*n*-valerate – gives excellent and interesting effects in Rum, Arak, Brandy, Cognac and Wine flavors, also the type called "Champagne" (often a winey variation of Apple-flavor for Gelatin desserts or Gelatin candy). It gives power and richness to the conventional esters used in such flavors, and it lends the much desired creamy-buttery note to Rum flavor, although it is by no means a key ingredient.

The author believes that the ester is not used in perfumery except for occasional application in artificial essential oils, etc.

Prod.: by direct esterification of *trans-2*-Hexenol with (*iso*-)Valeric acid, preferably under azeotropic conditions.

*iso*-Valerate: available 1965-1968.

*n*-Valerate: occasionally produced since 1967.

156-17;
(samples: Compagnie Parento, Inc.).

## 1634: 2-HEXOXYACETALDEHYDE DIMETHYLACETAL

*beta*-Hydroxyacetaldehyde dimethylacetal, hexylether.

$C_6H_{13}—O—CH_2—CH(OCH_3)_2$

$C_{10}H_{22}O_3 = 190.29$

Colorless, slightly oily liquid. B.P. 209° C.

Almost insoluble in water, soluble in alcohol and oils. Fairly soluble in Propylene glycol.

Moderately powerful, but pleasantly fresh-green, vegetable-juicy odor with a faintly fruity undertone. Overall a truly new green odor, yet reminiscent of natural materials, juicy flowerstalks, etc.

This Acetal was introduced only very recently (1967) by Fritzsche Bros., Inc. as a selected member of an extensive series of Oxyaldehydes and their Acetals.

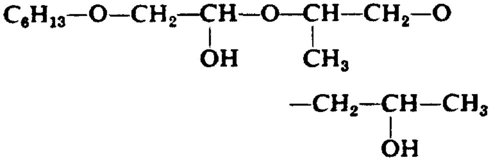
It is finding increased use in perfume compositions, particularly as part of new and interestingly refreshing topnotes. As a partly sweet-green, partly fruity-green odor, it is extremely versatile, and its lack of high pungency makes it easier to apply in experimental perfumery. The concentrations used may often exceed 1 %, in rare cases considerably higher, depending upon the type of basic fragrance. This Acetal is particularly interesting in Muguet, Hyacinth, Geranium, Narcisse, etc. but it can be used in many non-floral types, too. With certain types of Citrus note, it gives unique freshness in Chypres and light Oriental bases.

The author feels that this Acetal will find extensive use in perfumery. It is not yet suggested for use in flavor compositions, but it is most conceivable that it can be approved for such use, and then find new applications in Apple, Gooseberry, Melon, and many vegetable types of flavor.

Prod.: (several methods) el. g. from Bromoacetal and Potassium hexylalcoholate.

(Sample: Fritzsche Bros. Co., Inc.).
Ref.: American Perfumer and Cosmetics, June 1967, vol. 82, pages 29-30.

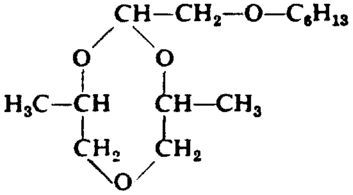
## 1635: 2-HEXOXYACETALDEHYDE DIPROPYLENEGLYCOL HEMIACETAL



$C_6H_{13}—O—CH_2—\underset{OH}{CH}—O—\underset{CH_3}{CH}—CH_2—O—CH_2—\underset{OH}{CH}—CH_3$

$C_{14}H_{30}O_5 = 278.39$

presumably with some of the cyclic acetal:



$C_{14}H_{28}O_4 = 260.38$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, fresh-green, vegetable type of odor of moderate to good tenacity.

This hemiacetal was introduced early in 1968 by Fritzsche Bros. Co. in addition to the Dimethylacetal previously marketed.

If anyone, who is excited about the Dimethylacetal, should find that its modest tenacity is a drawback, there is a good chance that the subject hemiacetal will satisfy his wishes.

It has a similar odor type, although somewhat sweeter, more Melon-like and less sharp-green than the Dimethylacetal. The manufacturer claims that it has more power and is more tenacious than the DMA, and adds that this is unusual. The human nose and olfactory system is notoriously poor and incorrect when it comes to comparative evaluation of odor "power", and the author feels that the good tenacity of the material is fairly easy to prove, while its power can be discussed as it is an extremely subjective question.

In any event, the Hemiacetal is a very

promising perfume chemical and it appears on the market at a time when the consumers are looking for novel fragrance notes. Besides, there is always a psychological aspect in the subconscious preference for an odor when it has a gentle but unquestionable relationship to edible and popular foods.

(See: Fritzsche Bros. Co. Inc., Bulletin of 8th April 1968).
(Sample: Fritzsche Bros. Co., Inc.).

## 1636: HEXYL ACETATE

*n*-Hexyl acetate.
Hexanyl ethanoate.

$CH_3(CH_2)_4CH_2—OOC—CH_3$

$C_8H_{16}O_2 = 144.22$

Colorless liquid. Sp.Gr. 0.87. B.P. 172° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Sweet fruity Berry-and-Pear-like odor, milder than Amyl acetate, less natural, slightly floral and green.

Sweet fruity taste reminiscent of berries (e. g. Cherry) and Pear, pleasant in concentrations below 40 ppm.

This ester is only rarely used in perfumery.

It finds some use in flavor compositions for imitation Apple, Cherry, Banana, Date, Gooseberry, Pear, Pineapple, Strawberry and various other berry or fruit complexes, Tutti-frutti, etc.

Concentrations are normally about 3 to 25 ppm in the finished product.

Hexyl esters are relatively rare in Nature, and are therefore somewhat more difficult to use in imitation fruit flavors than the common or "natural" esters. Hexyl acetate however, is probably one of the more popular and useful Hexyl esters.

Prod.: by direct esterification of *n*-Hexanol with Acetic acid under azeotropic conditions, or with Acetic anhydride.

G.R.A.S. F.E.M.A. No.2565.

4-61; 26-572; 33-500; 34-1230; 66-586; 86-59; 90-203; 140-134; 103-94; 160-770; B-II-132;

## 1637: iso-HEXYL ACETATE

*2*-Methylpentan-*5*-yl acetate.

$(CH_3)_2CH(CH_2)_3—OOC—CH_3$

$C_8H_{16}O_2 = 144.22$

Colorless slightly oily liquid. B.P. 160° C.

Practically insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Sweeter and fruitier than Amyl acetate, less harsh. Not quite as floral as Hexyl acetate, and not as "berry-like".

The flavor is sweet and fruity, rather nondescript, but has a remote resemblance to Apple and Pear.

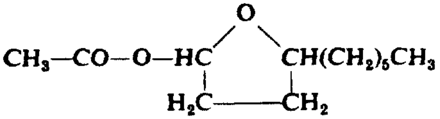
Has been suggested for use in flavor compositions, but does not seem to perform as well as *n*-Hexyl acetate, since the *iso*-Hexyl acetate is less versatile and less reminiscent of any natural fruit.

The author is not aware of any use of this ester in perfumery.

Prod.: by direct esterification of *2*-Methylpentanol-*5* with Acetic acid under azeotropic conditions.

26-572; 31-122; B-II-133;

## 1638: 2-HEXYL-4-(or-5)-ACETOXY TETRAHYDROFURAN



$C_{12}H_{22}O_3 = 214.31$

Colorless liquid. Slightly soluble in water, soluble in alcohol and oils.

Sweet, floral-fruity odor with caramellic "jam"-like note and good tenacity.

Sweet fruity and relatively powerful taste, not resembling any single fruit, but of an overall Peach-Apricot-like type.

This material has, to the author's knowledge, no application in perfumery. It could be on account of its rather poor stability in mildly alkaline media, while the material is quite stable under normal acid conditions.

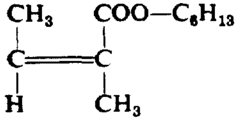
Is is used in trace amounts in fruit flavors as a fortifier or interesting background note. If it were more stable, it could be of interest in dentifrice flavors, too.

G.R.A.S. F.E.M.A. No.2566.

(See lit.: 69-164).

## 1639: n-HEXYL ANGELATE

*n*-Hexyl-*cis-2*-methyl crotonate.
*n*-Hexyl-*cis-2*-methyl-*2*-butenoate.
*n*-Hexyl-*cis-2,3*-dimethylacrylate.



$C_{11}H_{20}O_2 = 184.28$

Colorless or pale straw-colored slightly oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, tealike and winey odor.

Herbaceous, fruity-winey taste in dilutions below 20 ppm.

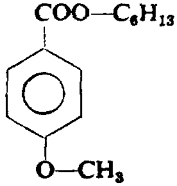
This ester, not very commonly offered to the trade, has found a little use in perfumery, mainly in the reproduction of certain essential oils. Until such time that Angelic and Tiglic acids can be produced separately at a very low cost, there is probably not much chance that this ester and other Angelates will become standard items on the perfumer's shelf. Furthermore, the Angelates are the less stable modifications of the two stereo-isomers, and Tiglates have accordingly become rather much in demand.

Prod.: by direct esterification of *n*-Hexanol with Angelic acid under azeotropic conditions.

90-224;

## 1640: HEXYL ANISATE

*para*-Methoxy hexylbenzoate.



$C_{14}H_{20}O_3 = 236.31$

Colorless, slightly oily liquid. Sp.Gr. 1.04. B.P. 290° C.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Mild Cherry-anisic, fruity-floral odor with some resemblance to Hawthorne and Heliotrope. Excellent tenacity.

Sweet anisic-Cherry-like flavor in dilutions below 40 ppm.

Of little more than academic interest, this ester may find some use in perfumery as a modifier for Heliotropine and Anisalcohol in herbaceous-floral, sweet fragrance types.

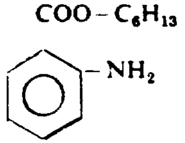
Apart from being a possible modifier in Vanilla imitation flavors, the ester has probably little or no application in food flavors.

Prod.: from *n*-Hexanol and Anisic acid by azeotropic type esterification.

34-681; 34-1231; 86-59;

## 1641: HEXYL ANTHRANILATE

*ortho*-Amino-*n*-hexylbenzoate.



$C_{13}H_{19}NO_2$ = 221.30

Colorless or pale straw-colored, slightly oily liquid. Sp.Gr. 1.03. B.P. 335° C.

Sweet, but very weak, fruity-floral odor with resemblance to Plum and Neroli. Excellent tenacity.

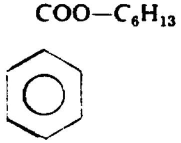
This ester is of very little interest to the perfumer and flavorist. Apart from being a fair fixative, its odor contribution to a fragrance composition, is neither powerful nor interesting. It is most conceivable that this ester will become obsolete if it is not already so.

Prod.: from *n*-Hexanol and Anthranilic acid by azeotropic type esterification. Also from Isatoic acid anhydride.

34-1231; 86-59;

## 1642: HEXYL BENZOATE

*n*-Hexyl benzoate.



$C_{13}H_{18}O_2$ = 206.29

Colorless liquid. Sp.Gr. 0.99. B.P. 272° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

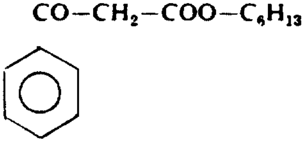
Woody-green, piney-balsamic odor with sweet-herbaceous undertones. The odor has been compared to that of "freshly decorticated Cypress twigs" (material ready for distillation).

This ester is an excellent modifier/blender for Labdanum, and a good companion wherever Labdanum is used: Balsamic-Ambre-Chypre-Fougère, etc., and it acts as a supporting fixative.

Prod.: by esterification of *n*-Hexanol with Benzoic acid under azeotropic conditions.

4-61; 34-1231; 86-57; 103-130;

## 1643: n-HEXYL BENZOYL ACETATE



$C_{15}H_{20}O_3$ = 248.33

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and warm-balsamic, herbaceous odor of good tenacity.

This ester, very rarely offered under its proper chemical name, finds use in perfume compositions as supporting note for Labdanum and other sweet-Ambre materials.

Its pleasant, ethereal-balsamic topnote blends very well with refined Labdanum products, with Amyl salicylate and Fougère bases, with Opopanax and Oriental fragrance types, with Styrax products, etc.

A number of aromatic esters are available with Labdanum-like notes, see also:

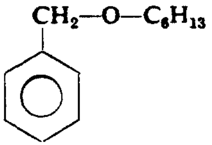
Ethyl-*3*-hydroxy-*3*-phenylpropionate, and Ethyl benzyl acetoacetate.

Prod.:

1) from Ethyl benzoate and Hexylacetate (or Hexyl acetoacetate) using Sodium ethoxide as condensing agent.
2) from Hexyl carbonate and Acetophenone.

## 1644: HEXYL BENZYL ETHER

Benzyl hexyl ether.
Benzyl hexyl oxide.
"Gardenia oxide" (this name is also used for Amyl benzyl ether).



$C_{13}H_{20}O = 192.30$

Colorless liquid. B.P. 245° C.

Insoluble in water, soluble in alcohol and oils.

Green-fruity, somewhat harsh-floral or slightly sharp-floral odor with a vague resemblance to Gardenia and Jasmin.

Suggested for use in low-cost Jasmin and Gardenia-type fragrances as a modifier for *iso*-Amyl benzyl ether and Benzyl esters in soap perfumes, etc. The Hexyl ether seems to lean more towards Gardenia and less to Jasmin with its greener note, but it is also more "hard" in its performance, with the all too well known "metallic" note of the Hexyl family. However, its power and tenacity could be utilized in soap and detergent perfumes, etc.

Prod.: by dehydration of a mixture of *n*-Hexanol and Benzyl alcohol. Also from Sodium hexylalcoholate and Benzyl chloride.

37-171; 86-59;

## 1645: HEXYL BUTYRATE

*n*-Hexyl-*n*-butanoate.

$CH_3(CH_2)_5—OOC(CH_2)_2—CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless mobile liquid. Sp.Gr. 0.87.
B.P. 208° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful, fruity, heavy odor, reminiscent not of one particular fruit, but of a "melange" of unripe fruits.

Probably of very little interest to perfumery, this ester finds some application in flavor compositions.

In trace amounts it introduces power and fresh notes in Strawberry, Cherry, Pineapple, Chocolate (or Cocoa) and in various berry and fruit complexes.

The concentration will normally be as low as 2 to 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2568.

Prod.: by direct esterification of *n*-Hexanol with *n*-Butyric acid under azeotropic conditions. Also from *n*-Hexanol and *n*-Butyric anhydride.

4-61; 33-732; 34-1230; 86-59; 95-181; 90-209; 103-114; 140-139;

## 1646: **HEXYL**-iso-**BUTYRATE**

*n*-Hexyl-*iso*-butanoate.

$CH_3(CH_2)_4—CH_2—OOC—CH(CH_3)_2$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Sp.Gr. 0.87. B.P. 199° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful, but rather harsh-fruity, nondescript type of odor, even less natural than the *n*-Butyrate.

The author believes that this ester is of very little interest to the perfumer or the flavorist. The *n*-Butyrate is likely to be preferred if at all this odor type is desirable.

Prod.: by direct esterification of *n*-Hexanol with *iso*-Butyric acid under azeotropic conditions. Also from *n*-Hexanol and *iso*-Butyric anhydride.

## 1647: iso-**HEXYL**-n-**BUTYRATE**

*iso*-Hexyl-*n*-butanoate.
*2*-Methylpentan-*5*-yl-*n*-butyrate.

$(CH_3)_2—CH—CH_2—CH_2—CH_2—OOC—$
$CH_2—CH_2—CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. B.P. 197° C.

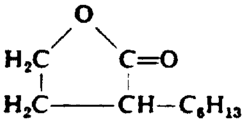
Sweet-fruity, but rather harsh, "chemical" odor with no obvious resemblance to any particular fruit.

Somewhat more powerful than the esters of *n*-Hexanol, this ester could be preferred for certain masking purposes, but the author can see no special advantage in the Aroma of this material as compared to the *n*-Hexyl esters for use in perfumes or flavors.

Prod.: by direct esterification of *2*-Methylpentan-*5*-ol with *n*-Butyric acid under azeotropic conditions.

## 1648: alpha-**HEXYL**-gamma-**BUTYROLACTONE**

a Decalactone.
Commercial Decalactone is usually *gamma*-Hexyl-*gamma*-butyrolactone.



$C_{10}H_{18}O_2 = 170.25$

Colorless or very pale straw-colored oily liquid. B.P. 251° C. Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Dry-fruity, unripe-Apricot-type odor with Ambre-like background.

The flavor in dilutions below 5 ppm is fairly pleasant, but has a somewhat confusing picture of Ambre-like or perfumey notes with Apricot-Peach admixture.

This lactone has been suggested for use in perfume compositions as a modifier for the more conventional lactones. It produces interesting variations in the fruity background notes of heavy Ambre-like perfumes, and it does not produce the overly sweet or heavy-fruity notes often derived from Undecanolide.

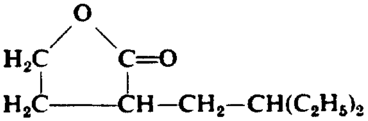
In the author's opinion, this lactone does not lend itself very easily to application in flavor compositions

Prod.: from *n*-Hexyl malonic ester and Ethylene oxide.

31-170; 86-59; 159-418;
See also: *gamma*-Decalactone,
*delta*-Decalactone,
and the next monograph.

## 1649: alpha-iso-HEXYL-gamma-n-BUTYROLACTONE

*alpha*-(*3*-Methylolpentane)-*gamma*-butyrolactone.
*alpha*-(Diethyl-ethyl)-*gamma*-butyrolactone.
a Decalactone.



$C_{10}H_{18}O_2 = 170.25$

Almost colorless oily liquid. B.P. 247° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

Fatty, green-musky or slightly animal-heavy odor. Overall not as pleasant as the *n*-Hexyl lactone. Some observers find a similarity to Costus, others find Ambre or Musk. It is apparent that the odor is more animal, less fruity or floral than that of the other isomers.

This lactone has found some use in perfumery as a modifier for Ambre-like notes, a mildly animal fixative, and a soft background odorant in various fragrance types, mostly the non-floral ones.

It blends excellently with Oakmoss, Galbanum, Labdanum, Costus, Ionones and Methylionones, and with many synthetic or natural Orris notes. At proper (low level) concentration, it may assist in creating the often wanted "powdery" notes in non-floral fragrances.

Prod.: from *iso*-Hexylmalonic ester plus Ethylene oxide.

31-170; 31-171; 86-59;

## 1650: HEXYL CAPROATE

*n*-Hexyl hexanoate.

$C_6H_{13}—OOC—C_5H_{11}$

$C_{12}H_{24}O_2 = 200.32$

Colorless, slightly oily liquid. Sp.Gr. 0.87. B.P. 245° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Fresh-vegetable-like, slightly fruity odor resembling that of Stringbeans (haricots verts), but slightly more "grassy".

Sweet-green, somewhat fruity taste, pleasant at concentrations below 20 ppm.

This ester finds a little use in perfumery as part of "green" notes, mostly in non-floral fragrance types. It blends very well with Galbanum and Oakmoss, and it gives interesting effects with Lavender, Clary Sage, Rosemary, etc.

The ester is probably more often used in flavor compositions, mainly in fruit flavors to add freshness and a touch of green note to various berry and fruit imitations flavors. It gives good effects in Strawberry, a flavor in which the Hexyl family plays an important role. Concentrations are usually as low as 2 to 10 ppm in the finished product.

Approved for use in food flavors by the American F.R.

Prod.: by direct esterification of *n*-Hexanol with Caproic acid under azeotropic conditions.

4-61; 34-1230; 86-59; 103-180;

## 1651: HEXYL CAPRYLATE

*n*-Hexyl-*n*-octoate.
*n*-Hexyl octylate.
*n*-Hexyl-*n*-octanoate.

$CH_3(CH_2)_5—OOC—(CH_2)_6—CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid. Sp.Gr. 0.87. B.P. 260° C.

Insoluble in water, soluble in alcohol and oils.

Oily-herbaceous, slightly green, condiment-like odor with sweet undertones.

In extreme dilution (lower than 5 ppm) this ester has a fairly pleasant fruity-herbaceous taste, reminiscent of sweet herbs, but at higher concentrations this impression is partly ruined by oily-animal notes.

The ester is rarely, or perhaps never, used in perfumery.

It finds a little use in flavor compositions where it adds green-sweet, herbaceous background to fruity or vegetable-fruity complexes.

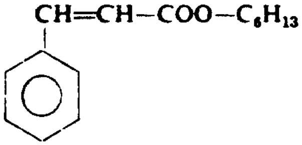
The concentration used is normally equivalent to 1 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2575.

Prod.: by direct esterification of *n*-Hexanol with Caprylic acid under azeotropic conditions.

34-1231; 86-59;

## 1652: HEXYL CINNAMATE



$C_{15}H_{20}O_2 = 232.33$

Almost colorless oily liquid. Sp.Gr. 1.00. B.P. 325° C.

Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Warm-herbaceous-balsamic odor with fruity-balsamic, yet somewhat dry and almost woody undertones. The odor has been compared to that of Cypress (twigs), but it has a somewhat sharper greenness.

This ester, not very commonly offered to the trade, finds a little use in perfumery to assist in producing the frequently desired "powdery" notes in Ambre type fragrances, or in the terminal notes of floral fragrances. It blends well with Styrax, Labdanum and the Methylionones, or with Mimosa, orrisy or woody notes.

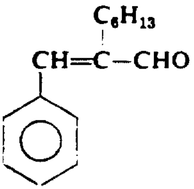
Prod.: by direct esterification of *n*-Hexanol with Cinnamic acid under azeotropic conditions.

It has also been prepared from Hexylacetate plus Benzaldehyde by condensation in the presence of Sodium or Magnesium Hexylalcoholate (at low temperature).

34-462; 34-1231; 86-59;

## 1653: HEXYL CINNAMIC ALDEHYDE

*alpha-n*-Hexyl cinnamal.
Jasmonal H.
Jasminolene.
H.C.A.
– and many trade names.



$C_{15}H_{20}O = 216.33$

Pale yellowish oily liquid. Sp.Gr. 0.95. B.P. 305° C.

Insoluble in water, Propylene glycol and Glycerin. Soluble in alcohol, miscible with oils.

Very mild, sweet-oily, slightly floral odor with a trace of herbaceous undertones.

The odor becomes considerably more floral and lively when the material is incorporated with more volatile material in a composition. If the aldehyde is old, poorly stored, or of initially poor quality, it may show fatty or rancid-oily notes which more or less ruin the olfactory picture of this excellent material.

Mild, sweet-oily-herbaceous and warm taste in dilutions below 10 ppm.

This aldehyde finds considerable use in perfume formulations for its rich floral and pleasant oily-herbaceous odor-contribution to Jasmin bases, Gardenia, Tuberose, Magnolia, etc. and in general as part of a floral theme in other fragrance types. There are many perfumers who find this aldehyde superior to Amylcinnamic aldehyde, and the author believes that many cases of objection to the Hexyl-cinnamic aldehyde can be traced back to lack of experience with a good grade of it, lack of olfactory proof that it does perform excellently. There are also indications that the infrequent use of such material can cause objections (or rejections) when older or deteriorated samples are evaluated for use. This aldehyde suffers the same drawback of poor stability as the Amylcinnamic aldehyde. It also suffers from the hazards of contamination with unsaturated (olefinic) aldehydes appearing as by-product in the process of making HCA. These aldehydes, particularly "Dioctenal" contribute unpleasant, fatty, rancid odor to the product, and their total absence is one of the principal prerequisites for a high-grade Hexyl cinnamic aldehyde.

The aldehyde finds a little use in flavor compositions, mainly for imitation Honey, and in various fruit and berry complexes.

The concentration used is normally about 0.1 to 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2569.

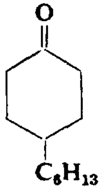
FCC-1964-833.

Prod.: by condensation of Benzaldehyde with Octanal (under alkaline conditions).

31-51; 31-57; 86-60; 93-150; 106-185; 156-27; U.S. patent (DuPont de Nemours No. 2102965 (1937).

## **1654:** n-**HEXYL-4-CYCLOHEXANONE**

*1*-Oxo-*4*-hexyl cyclohexane.
*para*-Hexyl-cyclohexanone.



$C_{12}H_{22}O = 182.31$

Colorless liquid. B.P. 247° C.

Insoluble in water, soluble in alcohol and oils.

A French registered patent of Bayer covers the manufacture of a series of *para*-Alkyl cyclohexanones from Hexyl and up.

Although the patent is nearly 30 years old, only a few of these ketones have become of any importance to the perfume industry. Some of these are still sold under trade names.

Most of these ketones have woody, woody-camphoraceous, sweet-camphoraceous or Orris-like odors, and they perform best in combination with Ionones, Cedarwood derivatives, etc. particularly for soap perfumes and other large volume preparations. The following two materials are closely related to subject ketone, and the *ortho*-isomer has been marketed under a trade name as a Vetiver-type chemical.

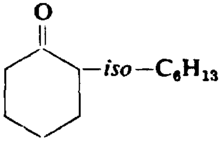
The *para-tertiary*-Butyl derivatives have already found some use in perfumery, and the *para-tertiary*-Amyl derivative is also a commercially available perfume chemical. Several *ortho*-isomers are also of perfumery interest.

Prod.: from *para*-Hexyl cyclohexanol by Chromic acid oxidation. (The alcohol is obtained by hydrogenation of the corresponding phenol).

31-99;

## **1655:** iso-**HEXYL-2-CYCLOHEXANONE**

*1*-Oxo-*2*-*iso*-hexyl cyclohexane.
*ortho*-*iso*-Hexyl cyclohexanone.



$C_{12}H_{22}O = 182.31$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Woody-Orris-like odor with earthy-minty, Vetiver-like undertones and good tenacity.

This ketone is commercially available under a trade name, and it is suggested for use in Vetiver compositions, in Chypre and Oriental fragrance types, in soap perfumes and in general as a supporting factor for Ionones, Sandalwood and Vetiver, Patchouli, Oakmoss and woody-mossy materials.

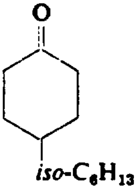
See also notes under previous monograph.

Prod.: by Chromic acid type oxidation of *ortho-iso*-Hexyl cyclohexanol, which is obtained by hydrogenation of *ortho-iso*-Hexyl phenol.

Parfumerie, Cosmetiques, Savons, August 1965 (Societe de Productions Documentaires, Paris VII').

## 1656: iso-HEXYL-4-CYCLOHEXANONE

*1*-Oxo-*4*-*iso*-hexyl cyclohexane.
*para-iso*-Hexyl cyclohexanone.



$C_{12}H_{22}O = 182.31$

White crystalline mass, melting at 33° C.

Insoluble in water, soluble in alcohol and oils.

Slightly Orris-like, mainly camphoraceous-minty odor of good tenacity and considerable radiance.

This ketone is probably the least interesting of a series, three of which are mentioned in this work (see previous two monographs).

Apart from general use as a "lifting" and powerful, stable ingredient in soap perfumes, there is probably not any strong interest in the material.

See comments under *para*-Hexyl cyclohexanone.

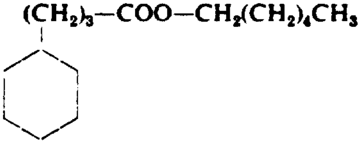
Prod.: by oxidation of *para-iso*-Hexyl cyclohexanol with Chromic acid. The alcohol is obtained from the corresponding phenol by catalytic hydrogenation.

Parfumerie, Cosmetiques, Savons, August 1965 (Société de Productions Documentaires, Paris VII').

See also: 31-99;

## 1657: HEXYL CYCLOHEXYL BUTYRATE

Hexyl cyclohexane butyrate.
Cyclohexane butyric acid, hexylester.



$(CH_2)_3-COO-CH_2(CH_2)_4CH_3$

$C_{16}H_{30}O_2 = 254.42$

Colorless oily liquid. Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity odor with green-herbaceous undertones.

This ester has been suggested for use in perfumes (and flavors), but does not seem to have become very popular or common.

The author is not aware of any important use of this ester, and it is only occasionally offered commercially to the perfume trade.

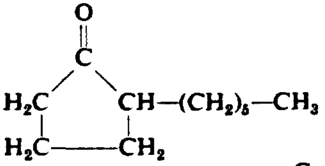
It could be compared to Allyl cyclohexyl butyrate, which is somewhat more common and regularly used in perfumes and – particularly – in flavors. The Hexyl ester does not produce the Pineapple-like flavor effects obtained with the Allyl ester, and the latter is somewhat more powerful.

Prod.: by direct esterification of *n*-Hexanol with Cyclohexane butyric acid under azeotropic conditions.

4-61;

## 1658: 2-HEXYL CYCLOPENTANONE

*alpha-n*-Hexyl cyclopentanone.
(Part of Dihydro-*iso*-jasmone).



$C_{11}H_{20}O = 168.28$

Very pale yellowish or almost colorless oily liquid.

Insoluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and diffusive, dry-floral, green-herbaceous odor with considerable resemblance to part of the natural Jasmin complex.

It is less spicy or Celery-like than Jasmone, more sharp-fruity or green, and not quite as powerful. Rather than considering it as a low-cost substitute for Jasmone, it would be better to use it as an individual fragrance material with effects of its own. It will lend considerable floral-herbaceous power to fragrances other than the typical floral ones, and it may participate in giving Jasmin effect when blended with suitable components.

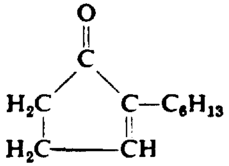
Prod.:

1) by condensation of Hexaldehyde and Cyclopentanone, followed by hydrogenation of the condensation product.
2) by hydrogenation of the reaction mixture from Lactonization of Undecylenic acid with Phosphoric or Polyphosphoric acid.

34-1211; 156-223;

## 1659: 2-n-HEXYL-2-CYCLOPENTEN-1-ONE

Sometimes called "Dihydrojasmone" (name is misleading).
Subject material is the chief ingredient in certain commercial products sold under the name of *iso*-Jasmone.
See monograph: *iso*-Jasmone, component A.



$C_{11}H_{18}O = 166.27$

Pale yellowish liquid, darker with age or after poor storage conditions.
Sp.Gr. 0.91. B.P. 241° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Powerful fruity-green, oily and somewhat floral odor of moderate tenacity.

This ketone is widely used in perfume compositions as a "floralizer" not only in Jasmin bases and related florals, but in general to introduce floral power with relatively small volume of ingredient. The subject material is capable of producing interesting and – at proper use level – pleasant topnotes, particularly in combination with fruity notes. It enhances Lavender, Lavandin and Clary Sage, and it seems to enrich other herbaceous materials, but it is also capable of dominating a fragrance to a degree of definite rejection if used at too high level, or without olfactory companionship.

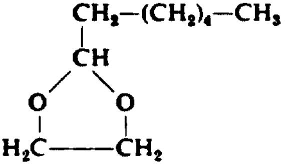
Perfumers do not generally agree which of the two common components of *iso*-Jasmone should be considered the "desirable" or preferred one.

Prod.: from Undecylenic acid with Phosphoric acid at low temperature.

4-61; 106-209; 156-220;
see also: Dihydrojasmone – and: Hexylidene cyclopentanone.

## 1660: 2-HEXYL-1,3-DIOXOLANE

Heptanal-ethyleneglycol-(cyclic)-acetal.
"Trefiol" (Noville Ess. Oil Co., Inc.).
Heptaldehyde glycolacetal.



$C_9H_{18}O_2 = 158.24$

Colorless oily liquid.

Insoluble in water, soluble in alcohol, Propylene glycol and oils.

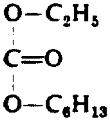
Powerful, sharp-herbaceous, fruity-weedy-green odor.

Suggested for use in perfume compositions, mainly Fougères, New Mown Hay, Clover, and in various modifications of Lavender and Sage, etc. The effect is somewhat less floral, more harsh than that of the next higher homologue, made from *1,2*-Propanediol, see monograph: Hexyl methyl dioxolane.

The subject cyclic acetal is commercially available under a number of trade names from several supply sources.

Prod.: by condensation of *n*-Heptaldehyde with Ethylene glycol.

## 1661: HEXYL ETHYL CARBONATE



$$\begin{array}{l} O-C_2H_5 \\ | \\ C=O \\ | \\ O-C_6H_{13} \end{array}$$

$C_9H_{18}O_3 = 174.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Refreshing, sweet-herbaceous odor with musky undertone.

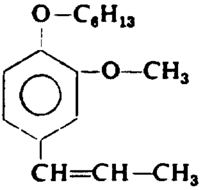
This ester is rarely offered under its proper chemical name, but it enters several perfume specialties as part of the ethereal-refreshing topnote, used in a great variety of perfumes – floral, herbaceous, citrusy, etc.

It seems to have a good ability of "mellowing" a fragrance, and introducing a "natural" note. In that respect, it resembles Ethyl acetoacetate, which, of course, does not nearly have the same tenacity as the title material.

Prod.: from Hexanol plus Ethyl alcohol with Phosgene (Carbonyl chloride).

## 1662: HEXYL-iso-EUGENOL

*iso*-Eugenol hexylether.



$C_{16}H_{24}O_2 = 248.37$

Viscous yellowish liquid. Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Very tenacious, balsamic-Vanilla-like odor of peculiar "green" sweetness, giving an overall impression of Cocoa or Chocolate rather than of Vanilla.

Suggested for use in perfume compositions, mainly as a fixative/modifier in heavy florals, Oriental fragrance types, etc.

It blends well with Peru balsam and its derivatives, Tolubalsam and the Cinnamates, Benzoin, Methylionones, Amylsalicylate and a great variety of sweet-floral or heavy odorants.

It is rather uncommonly offered to the trade, and it is unlikely that it will become very popular unless it can be brought on the market at a competitive cost and in steady supply.

Prod.: from Eugenol and *n*-Hexyl bromide in alcoholic alkaline solution, followed by Isomerization with strong Potassium hydroxide in alcohol.

7-206; 34-1115; 86-74;

## 1663: HEXYL FORMATE

*n*-Hexyl methanoate.

$CH_3(CH_2)_5—OOC—H$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. Sp.Gr. 0.89.
B.P. 155° C.

Slightly soluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Strongly diffusive, ethereal-fruity odor, refreshingly green and reminiscent of unripe Plums and Apples.

Sweet, green-fruity taste in dilutions below 100 ppm. Not very powerful flavor.

This ester is used mostly in flavor compositions. Its application in perfumes – if any – is limited to traces in topnote compositions and in reconstructed essential oils (Geranium, Lavender, etc.).

Hexyl formate is used quite widely in fruit flavors for imitation Apple, Cherry, Gooseberry, Lemon, Orange, Pineapple, Plum, Strawberry, Raspberry, etc. and in various fruit complexes, Tutti-frutti compositions, etc.

The concentration used is normally about 10 to 50 ppm in the finished product.

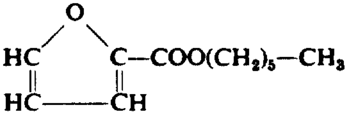
G.R.A.S. F.E.M.A. No.2570.

Prod.: by direct esterification of *n*-Hexanol with Formic acid, e. g. in presence of Acetic anhydride, or under azeotropic conditions.

4-62; 26-574; 31-126; 31-135; 34-1230; 86-60; 160-1000; B-II-22;

## 1664: n-HEXYL FUROATE

Hexyl-2-furoate.
Hexylfuran-*alpha*-carboxylate.
Pyromucic acid, *n*-hexylester.



$C_{11}H_{18}O_3 = 196.25$

Colorless or pale straw-colored liquid.
B.P. 252° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar fruity-earthy, yet sweet and Pear-like odor with a trace of fungus-like undertone.

Sweet, herbaceous-fruity, Mushroom-like flavor in extreme dilution.

This ester is – to the author's knowledge – exclusively used in flavor compositions, not in perfumery.

It is added in mere traces to imitation Coffee, Maple, Mushroom and various Nut-flavor compositions to introduce the sweet-earthy, yet fruity freshness that characterizes the natural products. Concentration is normally as low as 0.2 to 0.3 ppm in the finished consumer product.

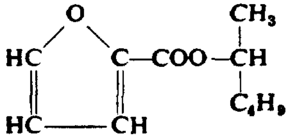
Prod.: by direct esterification of *n*-Hexanol with 2-Furoic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2571.

86-60;

## 1665: secondary-HEXYL FUROATE

Methyl-*n*-butylcarbinyl-2-furoate.



$C_{11}H_{18}O_3 = 196.25$

Colorless or pale straw-colored liquid.

Practically insoluble in water, soluble in alcohol and oils.

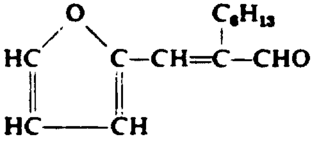
Dry-herbaceous, somewhat musty-metallic odor with fruity-earthy undertones, not nearly as pleasant as the *n*-Hexylester, and not as mushroom-like.

Although this ester has been mentioned as a perfume material, the author doubts that it has or will have any importance as such in the future. It may have a small academic interest in the systematic study of relationship between olfactory effect and chemical structure.

Prod.: by direct esterification of *secondary*-Hexanol with *2*-Furoic acid under azeotropic conditions.

## 1666: alpha-HEXYL FURFURACROLEIN

*alpha-n*-Hexyl-*beta-2*-furylacrolein (correct name).



$C_{13}H_{18}O_2 = 206.29$

Viscous yellowish oil. Sp.Gr. 0.98.
B.P. 248° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Mild, green-herbaceous odor with sweet-spicy undertones and a vague resemblance to Labdanum.

This aldehyde, very rarely offered commercially under its proper chemical name, was developed as a member of a series of aldehydes parallel to the alkylsubstituted Cinnamic aldehydes. It was the intention to find new aldehydes from Furfural, perhaps more interesting than those from Benzaldehyde.

The subject aldehyde is probably one of the more interesting of the series, but is relatively unstable and cannot compete with Hexyl- or Amylcinnamic aldehydes with respect to floral effect. However, it does contribute some interesting notes of its own, and blends very well with Labdanum, Benzoates, Cinnamates, the Eugenols, Amylsalicylate and many other heavy non-floral items.

Prod.: by Claisen type condensation of Furfural with Octanal.

31-40; 93-150;

## 1667: HEXYL HEPTOATE

*n*-Hexyl-*n*-heptanoate.
Hexyl heptylate.

$CH_3(CH_2)_5COO—C_6H_{13}$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 260° C.

Insoluble in water, soluble in alcohol and oils.

Fresh-green, but rather weedy, more sharp-sour-green than ordinary leafy odor, yet with sweet-juicy undertones. The green notes have been compared to those of freshly cut stems of hollyhock. Other observers find a Violet-leaf note. The overall impression is that of a rather unpleasant greenness, from a perfumery point of view.

The subject ester has been suggested for use in perfume compositions. The author feels, however, that there is little, if any, place for this fragrance picture in perfumery. Rare applications may include those of artificial essential oils, or novel notes in green topnote complexes.

Prod.: by direct esterification of *n*-Hexanol with *n*-Heptanoic acid under azeotropic conditions.

34-1231; 35-61; 86-60;

## 1668: n-HEXYL-n-HEPTYL ETHER

Heptylhexylether.

$C_6H_{13}—O—C_7H_{15}$

$C_{13}H_{28}O = 200.37$

Colorless oily liquid. Sp.Gr. 0.80.
B.P. 240° C.

Insoluble in water, soluble in alcohol and oils.

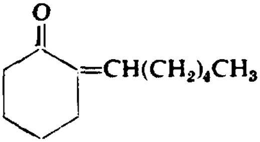
Rich, leafy, Hyacinth-green odor, reminiscent of cut stems of Bluebell, and also – remotely – of Galbanum.

This ester has been suggested for use in perfume compositions, and it could find a good place in Hyacinth, Lilac, Appleblossom, Wistaria, etc. and in modest concentration in a multitude of floral and non-floral compositions. It will lend power and stability, rich undertones in herbaceous fragrances (it makes "thin" Lavender compositions smell richer, etc.) but its overall odor picture is not overly pleasant. It happens to resemble Hyacinth, but Hyacinth happens to be a fragrance classified by many laypeople as an utmost "chemical" odor, even if it reproduces the natural fragrance very accurately. The concentration usable is therefore rather limited.

Prod.: by dehydration of the mixed alcohols Hexyl- and Heptyl-. It has also been produced from Hexylbromide plus Sodium heptyl-alcoholate.

4-59; 31-144; 35-60; 37-176;

## **1669:** 2-n-**HEXYLIDENE CYCLOHEXANONE**-1



$C_{12}H_{20}O = 180.29$

Pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, green-floral, refreshing odor, reminiscent of Cyclamen and vegetables.

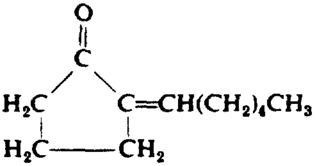
This ketone was developed in search of less expensive versions of 2-Hexylidene cyclopentanone (see next) in the *iso*-Jasmone family. It is rarely offered under its proper name, and it is mostly used in combination with related ketones for powerful floral effects in soap perfumes.

Prod.: by condensation of Hexanal with Cyclohexanone.

28-534;
see also: 156-223;

## **1670:** alpha-**HEXYLIDENE CYCLOPENTANONE**

*2-n*-Hexylidene cyclopentanone.
(This ketone forms part of most commercial products sold under the name "*iso*-Jasmone").



$C_{11}H_{18}O = 166.27$

Pale yellowish oily liquid.
B.P. 240° C. Sp.Gr. 0.91.

Insoluble in water, soluble in alcohol and oils.

Powerful warm-floral and green-fruity odor with spicy-herbaceous undertones. Its topnote may appear rather sharp, but in dilution it becomes distinctly fruity-floral with a vegetable note.

This ketone, mostly offered in the shape of a component of a commercial product, is used extensively in perfumes as a floralizer, not only in Jasmin and related florals, but generally – although in concentrations of 2% or less – as a powerful ingredient to assist in creating topnotes and diffusive power in the fragrance. It may also form part of green or fruity topnotes as a modifier and softening material.

This ketone is considered as the less desirable isomer in the types of *iso*-Jasmone consisting of a mixture of several ketones. The more desirable ketone is Hexyl cyclopentenone, in which the double bond is located in the ring system, not in the side chain. Jasmone (*cis*-) has a double bond in the ring and one in the side chain, besides having a separate Methylgroup attached to the ring with the Pentenyl sidechain next to the ketone group.

It is also used in flavors where it can introduce very interesting effects at very low concentration. It gives lift and power to many fruit flavors, Peach and Plum in particular, Tutti-frutti, etc. and is used in many different types, such as Mint flavors for dentifrice and mouthwash preparations, in soft drinks etc.

G.R.A.S. F.E.M.A No.2573.

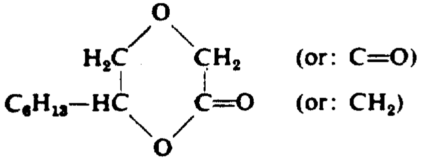
Prod.:

1) from Hexaldehyde and Cyclopentanone by condensation.
2) French patent No. 779789 (Givaudan (1935).
3) from Undecanolide and Polyphosphoric acid.

31-85; 86-60; 156-223;
see also: *iso*-Jasmone (monograph).

## 1671: 2-HEXYL-5-(or 6-)-KETO-1,4-DIOXANE

*delta*-Lactone of Hexylhydroxyethoxyacetic acid.



$C_{10}H_{18}O_3 = 186.25$

Colorless or very pale straw-colored liquid.

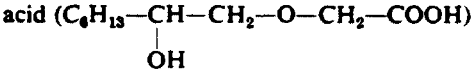
Slightly soluble in water, soluble in alcohol and oils. Fairly soluble in Propylene glycol.

Powerful, sweet, nut-like, creamy odor, in high concentration unpleasantly musty-musky, in extreme dilution pleasantly oily-creamy with nutlike notes.

The taste is sweet buttery-creamy in concentrations below 10 ppm.

This rare Lactone is used in flavor compositions, almost exclusively for Milk and Cream flavors, mainly intended for baked goods, candy and desserts. Concentrations are normally very low, up to about 5 ppm in the finished product.

Prod.: from Hexyl hydroxyethoxyacetic



acid $(C_6H_{13}-\underset{\textstyle OH}{\underset{|}{CH}}-CH_2-O-CH_2-COOH)$

by Lactonization.

G.R.A.S. F.E.M.A. No.2574.

## 1672: HEXYL LAURATE

*n*-Hexyl dodecanoate.
*n*-Hexyl dodecylate.

$C_6H_{13}$—$OOC(CH_2)_{10}CH_3$

$C_{18}H_{36}O_2 = 284.49$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 326° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Very mild oily odor. In the author's opinion, of very little interest to the perfumer.

This ester may find use in a few types of floral fragrance or artificial flower absolutes, e. g. Tuberose and similar types, where it can assist in producing oily-waxy "petal"-like notes in the floral picture. It has some advantage over Lauryl alcohol and its acetate (both occasionally used for similar purposes) in that the subject ester is much longer lasting, and does not tend to introduce an odor of its own or an "oxidized" note, which often happens with Lauryl alcohol.

Produced by direct esterification of *n*-Hexanol with Lauric (Dodecanoic) acid under azeotropic conditions.

## 1673: n-HEXYL MERCAPTAN

*1*-Hexanethiol.
*primary-n*-Hexylmercaptan.

$CH_3(CH_2)_4CH_2{-}SH$

$C_6H_{14}S = 118.24$

Colorless liquid. Sp.Gr. 0.85. B.P. 151° C. Insoluble in water, soluble in alcohol and oils.

Extremely powerful and diffusive odor. At concentrations near 0.1% in Diethyl phthalate, one can barely endure the evaluation and detect a striking similarity to the odor of "firecrackers", or recently extinguished matches, etc. In other words, a "burnt, sulfuraceous odor".

Mainly of academic interest, this material has occasionally found use in that special branch of perfumery which could be classified as "industrial odors". It has become fashionable not only to spray vaporized imitation flavor (of "newly baked bread") in the bread- and pastry department in supermarkets, in order to attract attention and appetite, but also in museum exhibits to add life to certain features or sceneries. Not so long ago, a London exhibit of the battle of Trafalgar in a museum was further enlived when vaporizers sprayed smoke, perfumed with "gunpowder odor" as the guns from the warships were "fired" for the show. This is one place where *n*-Hexyl mercaptan could be used with excellent effect.

Scientists have calculated that 10 grams of this material would be sufficient to odorize so much air that every human being on earth could smell it. Many scientists assume that a 50 ml. inhalation is average for a smelling sensation. The author of this work feels that the figure should be smaller.

A great number of Alkyl mercaptans (Alkane thiols) have been produced, and a commercial grade (mixture) of Amyl mercaptans is known under the name "Pentalarm" as a warning odor to be added to odorless household gas for safety purposes.

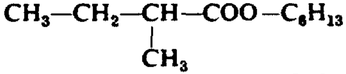
Prod.:

1) *from n-Hexylbromide* plus Potassium hydrosulfide in alcohol.
2) from Hexanol vapors plus Hydrogen sulfide gas over Thoria catalyst at 400° C.

26-574; 86-60; 160-1034; B-I-408;

## 1674: HEXYL-2-METHYLBUTYRATE

*2*-Methylbutanoic acid, *n*-hexylester.



$CH_3{-}CH_2{-}\underset{\displaystyle CH_3}{\underset{|}{CH}}{-}COO{-}C_6H_{13}$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils.

Powerful, fresh-green fruity odor. Overall somewhat sharp in its note.

Sweet, fruity-green taste, reminiscent of unripe Strawberries.

This ester, only recently commercially available, is used in various artificial essential oils, mainly Lavender, Lavandin, Peppermint and Spearmint.

It is also used in imitation Strawberry flavor in minute quantities.

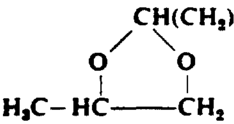
A large number of esters of *2*-Methylbutanoic acid have been prepared experimentally, particularly since many such esters have been identified in natural products.

G.R.A.S.

Prod.: by direct esterification of *n*-Hexanol with *2*-Methylbutanoic acid under azeotropic conditions.

## 1675: 2-HEXYL-5-METHYL-1,3-DIOXOLANE

*5*-Methyl-*2*-hexyl-*1,3*-dioxolane.
Heptanal-*1,2*-propanediol-(cyclic)-acetal.
Heptaldehyde propyleneglycol acetal.



$C_{10}H_{20}O_2 = 172.27$

Almost colorless oily liquid. Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful, fruity-green, intensely sweet and diffusive odor, reminiscent of fruits and vegetables.

This material, privately prepared, is suggested for use in perfume compositions, particularly in modern fragrances for household products, where novel fresh notes are desirable, room sprays, detergent fragrances, hair spray perfumes, etc. as well as a minor ingredient in herbaceous perfumes and in larger proportions in Fougères, etc.

This cyclic acetal blends very well with Coumarin, Lavender, Lavandin, Rosemary, Geranium, Citronellol, etc. in a great variety of fragrance types. It is quite penetrating and the use level may be as low as 1 to 3% under normal circumstances, while it can be as high as 4-8% in particularly powerful, fresh fragrance types, "outdoor" odors, etc.

Prod.: by "cold" condensation of *n*-Heptaldehyde with *1,2*-Propylene glycol under continuous removal of condensation water.

SA – private experiments 1961.
See also: *2*-Hexyl-*1,3*-dioxolane.

## 1676: HEXYL PELARGONATE

*n*-Hexyl nonanoate.
*n*-Hexyl nonylate.

$CH_3(CH_2)_4CH_2—OOC—C_8H_{17}$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid. Sp.Gr. 0.89.
B.P. 265° C.

Insoluble in water, soluble in alcohol and oils.

Winey-Cognac-like, somewhat oily, green-nut-like odor. Not as fatty or sour-oily as the Caproate or the Caprylate, overall sweeter.

Oily-Brandy-like, slightly fruity-sweet taste in dilutions lower than 10 ppm.

This ester finds a little use in flavor compositions as a component of imitation Cognac, Brandy, etc. and occasionally in fruit complexes, mainly Apple.

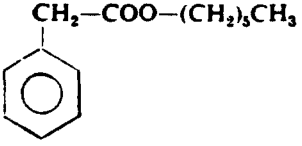
It is, to the author's knowledge, not used in perfumery.

Prod.: by direct esterification of *n*-Hexanol with Nonanoic (Pelargonic) acid under azeotropic conditions.

35-515; 34-1231; 86-60; 140-143;

## 1677: HEXYL PHENYLACETATE

*n*-Hexyl-*alpha*-toluate.



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid. Sp.Gr. 1.01.
B.P. 262° C.

Insoluble in water, soluble in alcohol and oils.

Sweet-green, fruity-winey odor, overall rather weak, but tenacious and with undertones that may vary from rosy to musky, according to origin of sample. The term "musky" is often used in panel descriptions of odors that appear weak, but are persistent and generally nondescript. Many observers will call such materials odorless.

This ester is occasionally used in perfume compositions, where sweet-green notes are called for, e. g. Acacia, Mimosa, Reseda, Violet (leaf), etc.

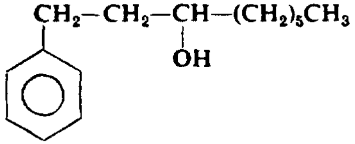
Its tenacity makes it fairly interesting as a modifier for lower Alkyl phenylacetates.

Prod.: by direct esterification of *n*-Hexanol with Phenylacetic acid under azeotropic conditions.

34-246; 34-1231; 86-60;

## 1678: HEXYL PHENYLETHYL CARBINOL

Phenylethyl hexyl carbinol.
9-Phenyl nonanol-7.



$C_{15}H_{24}O = 220.36$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Musty-rosy, mainly woody, and rather dry odor of moderate tenacity.

This alcohol has been suggested for use in perfume compositions. It is rarely, if ever, offered under its proper chemical name. Its peculiar, not immediately attractive odor requires quite some assistance from other odorants in order to produce pleasant effects. It will in most cases be limited to woody and harsh-rosy fragrances, e. g. soap perfumes, where the stability of this carbinol can be utilized with some advantage.

Prod.:

1) by Grignard type reaction on Phenylacetaldehyde with Hexyl Magnesium bromide.
2) by hydrogenation of Hexyl phenylethyl ketone.

4-62;

## 1679: n-HEXYL PROPIONATE

*n*-Hexyl propanoate.

$CH_3(CH_2)_5—OOC—C_2H_5$

$C_9H_{18}O_2 = 158.24$

Colorless liquid. Sp.Gr. 0.87. B.P. 180° C.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Peculiar sweetish-sour, almost "earthy" odor, resembling the odor of overripe fruit on the ground, with sweet-earthy-herbaceous notes. Some observers have described the odor as resembling that of "a steaming tropical atmosphere".

Sweet, metallic-fruity, almost "fermented" taste in dilutions lower than 50 ppm.

This ester is used in flavor compositions mainly for imitation Cocoa or Chocolate and in a few types of fruit flavor.

The concentration used is normally about 5 to 25 ppm in the finished product.

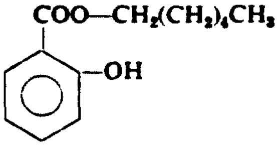
G.R.A.S. F.E.M.A. No.2576.

Prod.: by direct esterification of *n*-Hexanol with Propionic acid under azeotropic conditions, or with Propionic anhydride.

33-620; 34-1230; 86-60; 90-206;

## 1680: HEXYL SALICYLATE

*n*-Hexyl-*ortho*-hydroxybenzoate.



$C_{13}H_{18}O_3$ = 222.29

Colorless oily liquid. Sp.Gr. 1.04.
B.P. 290° C.

Practically insoluble in water, soluble in alcohol and oils.

Very faint, sweet-herbaceous and floral odor with dry-bark-like green undertones, sometimes referred to as "Witch-Hazel-odor". Poorer grades of this ester may be responsible for odor descriptions including the terms "phenolic" or "ink-like" (which also refers to "phenolic" in a secondary way) or "metallic". Pure Hexyl salicylate (with no free Phenolate other than the esterified Salicylic acid) has a definitely floral odor.

Although this ester in no way is a substitute for Amylsalicylate, is does have similar characteristics. Its inevitably higher cost has put a limit to its popularity, and the fact that imperfect distillation technique produced off-odor high-boiling materials up until a few years ago, also contributed to the lack of interest in many such materials.

Hexyl salicylate is used in a number of low-cost and medium-cost fragrance types as a modifier for the Amyl ester, or as a variation in floral or herbaceous-floral fragrances. Its tenacity is excellent and its odor comes to full perception when the ester is blended with more volatile components in a fragrance. It blends well with Labdanum, Coumarin, the Lavender oils or Rosemary, and it gives interesting effects in Carnation, Fougere, Chypre etc.

Prod.: by direct esterification of *n*-Hexanol with Salicylic acid under azeotropic conditions.

4-62; 34-789; 34-1231; 86-60; 103-181;

## 1681: n-HEXYL THIOGLYCOLATE

*n*-Hexyl-*2*-mercaptoethanoate.

$C_6H_{13}—OOC—CH_2—SH$

$C_8H_{16}O_2S$ = 176.28

Almost colorless oily liquid. Sp.Gr. 0.99.

Practically insoluble in water, soluble in alcohol and oils.

Green-fruity, almost medicinal or woody odor, vaguely resembling that of Blackcurrant. Traces of free Hydrogen sulfide – usually present in poor grade acids and esters – will completely ruin this odor picture.

Some observers find the odor animal, but the author is inclined to believe that such notes may derive from sulfide traces.

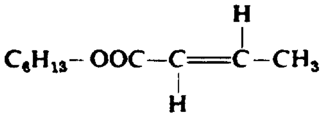
In spite of mention in the perfumery literature, this ester has probably very little, if any – interest to the creative perfumer. The author believes that this material has only academic interest.

Prod.: by direct esterification of *n*-Hexanol with Thioglycollic acid under azeotropic conditions.

34-1245;

## 1682: HEXYL TIGLATE

Hexyl tiglinate.
*n*-Hexyl-*trans*-*2*-methyl-*2*-butenoate.
*n*-Hexyl-*trans*-*alpha*-*beta*-dimethylacrylate.



$$C_6H_{13}-OOC-\underset{H}{C}=\overset{H}{C}-CH_3$$

$C_{11}H_{20}O_2$ = 184.28

Colorless liquid. Insoluble in water, soluble in alcohol and oils.

Pleasant, sweet-green, oily-herbaceous and slightly winey odor, reminiscent of unripe berries or unripe Plums.

Sweet-green, winey-fruity taste resembling that of unripe Blackcurrant.

This ester finds a little use in perfumery as ingredient in novel green type topnotes and in fresh smelling "natural" or "outdoor" odors for Colognes and sprays.

Its main use is, however, in flavor compositions, where it may introduce freshness to fruity and green-fruity compositions of many types. It gives richness to Apple flavor and Apricot or Mango, it supports the ethereal and light notes in Gooseberry and Strawberry, and it lends a natural "skin"-aroma to Plum flavors, etc.

For the skilled flavorist, this ester is a material with a multitude of possibilities.

Prod.: by direct esterification of *n*-Hexanol with Tiglic acid under azeotropic conditions.

90-224;
(sample: Fritzsche Bros., Inc. 1967).

## 1683: HEXYL UNDECYLATE

*n*-Hexyl undecanoate.

$C_6H_{13}$—$OOC(CH_2)_9CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid. B.P. 285° C.
Sp.Gr. 0.88.

Insoluble in water, soluble in alcohol and oils.

Very mild, earthy-root-like, mossy, mildew-like or slightly fungal odor. Some observers find the odor reminiscent of Parsnip.

The very peculiar and not very attractive odor of this ester limits its use to that of a trace or small component in certain woody or mossy-woody odor types as a modifier for Oakmoss products, Vetiver, etc. but this material is, in the author's opinion, not exactly needed in a perfume laboratory.

Prod.: by direct esterification of *n*-Hexanol with Undecylic acid under azeotropic conditions.

35-854; 103-181;

## 1684: n-HEXYL-n-VALERATE

*n*-Hexyl-*n*-pentanoate.
(Commercial material is often: *n*-Hexyl-*iso*-valerate, see next monograph).

$C_6H_{13}$—$OOC(CH_2)_3CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. B.P. 224° C. Sp.Gr. 0.87.

Insoluble in water, soluble in alcohol and oils.

Heavy-fruity odor reminiscent of unripe Apples, but with a musky undertone and sweetness. Overall less natural, less pleasant than the *iso*-Valerate.

This ester is occasionally used in perfumery as a trace additive usually where fruity notes need a "rounding off" or "mellowing", for which purpose the Valerate is notoriously useful – in the hands of the experienced perfumer.

The ester is rarely used in flavor compositions. The *iso*-Valerate is normally preferred for fruit and tobacco flavors, etc.

Prod.: by direct esterification of *n*-Hexanol with *n*-Valeric acid under azeotropic conditions.

5-238; 7-206; 86-60;

## 1685: n-HEXYL-iso-VALERATE

*n*-Hexyl-*iso*-pentanoate.
(Sometimes commercially called: Hexyl valerate).

$CH_3(CH_2)_5—OOC—CH_2—CH(CH_3)_2$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Sp.Gr. 0.87. B.P. 215° C.

Insoluble in water, soluble in alcohol and oils.

Somewhat pungent-fruity, "unripe"-fruity, slightly herbaceous, but rich and natural odor with a dry tobacco-leaf-like undertone.

Sweet-green, heavy fruity, slightly herbaceous taste in dilutions lower than 20 ppm.

This ester is used in perfume compositions, normally in traces only, to add heavy-fruity or tobacco-like herbaceous effects to Oriental fragrance types, Fougères, Chypres, etc., and to give – in minute traces – interesting top-notes upon delicate floral bases such as Muguet or Lilac, in higher amounts in Hyacinth. The musky-tobacco-like effect is useful along with Opopanax or Phenylacetates in Oriental types.

Traces are used in flavor compositions to "round-off" heavy fruity complexes, or in tobacco flavors, etc.

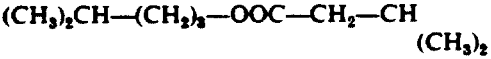
G.R.A.S.

Prod.: by direct esterification of *n*-Hexanol with *iso*-Valeric acid under azeotropic conditions.

33-932; 34-1231; 103-123;

## 1686: iso-HEXYL-iso-VALERATE

*2*-Methylpentan-*5*-yl-*beta*-methylbutyrate.
*iso*-Hexyl-*iso*-pentanoate.



$(CH_3)_2CH—(CH_2)_3—OOC—CH_2—CH(CH_3)_2$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Sp.Gr. 0.86. B.P. 208° C.

Insoluble in water, soluble in alcohol and oils.

Fruity, pungent odor with little or no resemblance to any particular fruit or other natural product. Its initial notes are rather sharp green, quite different from the odor of the common isomers.

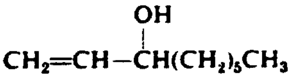
Although suggested for use in fruit flavors, this ester has probably very little importance as such.

Prod.: by direct esterification of *2*-Methylpentanol with *iso*-Valeric acid under azeotropic conditions.

4-62;

## 1687: HEXYL VINYL CARBINOL

"Homo-Mitsutake-alcohol".
Nonen-*1*-ol-*3*.
*8*-Nonen-*7*-ol.
Vinyl hexyl carbinol.
Androl.



$CH_2=CH-CH(OH)(CH_2)_5CH_3$

$C_9H_{18}O = 142.24$

Colorless oily liquid. B.P. 198° C.
Sp.Gr. 0.85.
Practically insoluble in water, soluble in alcohol and oils.

Powerful, oily-green creamy-waxy odor with a discrete undertone of peppery-earthy-mushroomy character. Moderate tenacity.

Sweet-earthy-oily taste with some resemblance to Mushroom.

This alcohol, a higher homologue of the more commonly used Amyl vinyl carbinol (*3*-Octen-*1*-ol), has found some use in perfumery as a fortifier for herbaceous or sweet-woody-earthy notes, e. g. Lavender, Oakmoss, Vetiver, Coumarin, etc. It has a fresher overall character than its lower homologue, and it may eventually convince more perfumers that it is more versatile and easier to apply.

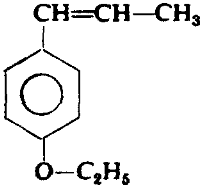
The alcohol finds some use in flavor compositions, mainly as a modifier for Amyl vinyl carbinol in Mushroom flavors.

Prod.: from Hexyl magnesium bromide plus Acrolein by Grignard reaction.

3-244; 87-486;
(Sample: Takasago Perfumery Co., Ltd.).

## 1688: HOMO ANETHOLE

"Ethyl anethole" (misleading name).
Paranol ethylether.
*1*-Propenyl-*4*-ethoxybenzene.
*para*-Propenyl phenethole.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Mild, sweet, herbaceous-spicy odor with a floral note. Overall weaker than Anethole, not typically anisic, and more floral.

Intensely sweet taste, but tends to be floral rather than herbaceous-spicy (anisic).

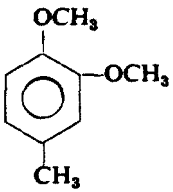
Suggested for use as a modifier for Anethole in flavor compositions, this ether has gained very little headway into the flavor laboratories, and the author doubts that this material will ever become a standard flavor item.

Prod.: by Ethylation of *para*-Propenylphenol with Diethylsulfate in aqueous alkaline solution.

31-147;

## 1689: HOMOCATECHOL DIMETHYLETHER

Homoveratrole.
*3,4*-Dimethoxytoluene.
*3,4*-Dimethoxy-*1*-methylbenzene.
*Creosol* methyl ether. (Name can be confused with *Cresol* methylether).



$C_9H_{12}O_2 = 152.20$

Colorless crystalline mass, melting at 21° C. to an almost colorless oily liquid.
Sp.Gr. 1.05. B.P. 220° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet, but tarry-medicinal odor of considerable diffusion and moderate tenacity. Undertones – under the tarry notes – are barely perceptible as sweet-floral and actually pleasant, reminiscent of terminal notes from Ylang Ylang oil.

Sweet, penetratingly medicinal taste, unless diluted below 5 ppm. Then almost Vanilla-like, balsamic-sweet, nut-like taste.

This ether is used in perfumery for smokey and medicinal effects as a variant from the conventional "medicinal" materials. It performs well with Ylang and Cananga oils, Labdanum and many Benzoates, *iso*-Eugenol, etc.

Although not recognized for flavor use in the U.S.A., this ether could possibly find use in Walnut and Nut flavor compositions. It has a pleasant effect with Oakmoss for such purposes.

Prod.:
1) by Methylation of Creosol with Dimethylsulfate in aqueous alkaline solution.
2) by Dimethylation of Homocatechol, which can be obtained from *para*-Cresol by electrolytic oxidation.

90-392;

## 1690: HOMOCETYL ALCOHOL

$CH_3(CH_2)_{16}OH$

$C_{17}H_{36}O = 256.48$

White leafy crystals. M.P. 54° C.
B.P. 292° C.

Insoluble in water, soluble in alcohol, miscible with oils.

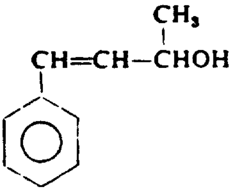
Very mild, Coconut-like, fruity-oily odor.

Although this material has been mentioned in perfumery literature and recommended for use in perfume compositions, the author is of the impression that this alcohol is used occasionally in cosmetic preparations, but rarely, if ever, forms part of a perfume composition with olfactory function.

4-62;

## 1691: HOMOCINNAMYL ALCOHOL

Methyl styryl carbinol (mainly *trans*-isomer).
*4*-Phenyl-*3*-buten-*2*-ol.
NOTE: This material is often called Methyl cinnamylidene carbinol, or:
*alpha*-Methyl-*gamma*-phenylallylalcohol, and it has therefore been confused with:
*alpha*-Methylcinnamic alcohol (see that monograph), and Cinnamylidene methyl carbinol (see that monograph).



$C_{10}H_{12}O = 148.21$

Colorless slightly viscous liquid.
B.P. 240° C. Sp.Gr. 1.00 (liquid).
Solidifies in the cold, melts at 34° C. Very pure material is an opaque crystalline mass.

Insoluble in water, soluble in alcohol and oils.

The author has used the title "Homocinnamyl alcohol" for this material, although it may not be the most common name for the subject chemical. However, confusion with the true *alpha*-Methylcinnamic alcohol encourages conspicuous separation of the two monographs.

Sweet and mild, fruity-balsamic, pleasantly floral odor of moderate tenacity.

This alcohol is used in flavor compositions for its pleasant sweet fruity note, applicable to almost any type of fruit composition. It is used mainly in Raspberry and Strawberry, but also in Peach and Plum. The taste in concentrations below 50 ppm is intensely sweet, fruity-jam-like, while at higher concentrations the floral theme seems to become dominating.

The concentration normally used is about 2 to 20 ppm in the finished product. The flavor is substantially improved in presence of proper food acids.

The author has no record of this material being used in perfume compositions, but it is very conceivable that it could be used in lipstick perfumes as a modifier to the Ionone-Methylcinnamate-Ethylmethylphenylglycidate theme, or in various Jasmin types as the fruity element with or without support from more conventional fruit odors.

G.R.A.S. F.E.M.A. No.2880.

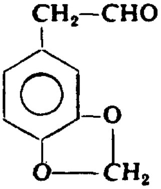
Prod.:

1) from Methyl magnesium iodide plus Cinnamic aldehyde.
2) by catalytic reduction of Benzylidene acetone in presence Palladium-Ferrous sulfate and Zinc atetate.

68-982; 163-224;

## 1692: HOMO HELIOTROPINE

Homopiperonal.
*3,4*-Methylenedioxy phenylacetaldehyde.
Homoprotocatechualdehyde methylene ether.
Sometimes called: "Liquid Heliotropine".



$C_9H_8O_3 = 164.16$

Colorless oily liquid. Darkens and resinifies upon exposure to air and daylight.
Sp.Gr. 1.26. B.P. 210° C. (under decomposition).

Insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Sweet and delicately floral-spicy odor, very reminiscent of Heliotrope, in some observers' opinion more so than Heliotropine itself.

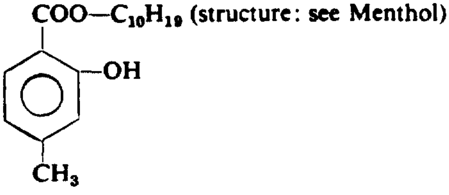
This Aldehyde has been suggested for use in floral perfume compositions as a modifier for Heliotropine, and in general as a floralizer and sweetener for delicate fragrance types. It has less of the "Cherry-pit" like odor than Heliotropine, but its chemical Nature makes it less accessible than the regular Heliotropine which can be produced at a fraction of the cost of producing the Homo heliotropine. With this high cost in mind, one can hardly see a bright future for this Aldehyde.

Prod.: from Safrole in an inert solvent by oxidation with Ozone, followed by reduction of the Ozonoid with Zinc in diluted Acetic acid.

7-207; 95-147;

## 1693: HOMO MENTHYLSALICYLATE

Menthyl-*4*-methylsalicylate.
"Menthylyl salicylate".
Menthyl-*meta*-cresotinate.
Menthyl-*gamma*-cresotinate.
Menthyl-2-hydroxy-*para*-toluate.



$C_{18}H_{26}O_3 = 290.41$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Faint "metallic" or "ink-like" odor, presumably due to traces of free phenol, other than the subject material. High-boiling salicylates have tendency to decompose during vacuum-distillation and break off traces of phenols.

This material, functionally a sunscreening agent, is mentioned mainly because it does have an odor, and it may enter functional products at such high concentration that its odor becomes a problem to the fragrance involved in the product.

When perfuming products containing this ester, due consideration should be paid to the fact that it is a high-boiling component and that its odor will mainly appear in the terminal notes of the fragrance which may be added to the cosmetic product. In other words, proper masking ability in the terminal notes are required for perfumes that accompany this ester in a functional product.

Prod.: by esterification (several methods) of *meta*-Cresotinic acid with Menthol (or an ester of Menthol).

155-359;

## 1694: HOMOQUINOLINE

Not a well-defined, single chemical.

The commercial product sold under this name is a mixture of Quinoline derivatives and homologues.

Average Mol. Wt. = $C_{13}H_{15}N$ = 185.27

Pale amber or pale brownish oily liquid.
Sp.Gr. 1.02.

Slightly soluble in water, soluble in alcohol and oils.

Very powerful and penetrating, diffusive and tenacious, sweet, heavy odor, with some resemblance to Honey, Castoreum, Oakmoss, Tobacco (cured, burnt Cigar tobacco), etc.

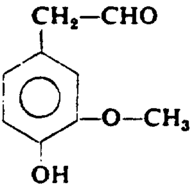
This material is used in minute traces in many different fragrance types, but primarily in heavy florals and Oriental types. It can also be used with interesting effects in Lilac and Sweet Pea, Honeysuckle and other florals, as well as in modern "Tabac" bases, Leather fragrances, woody bases, etc.

It is possible that its unusual power and tenacity has scared many perfumers from experiments, and it is true that careless handling of the item in the perfume laboratory could cause serious air-odor contamination or, in the better cases, some harsh words from the perfumer next door. But if used and operated in the proper dilution, this material can be more versatile and interesting than most of the conventional Quinoline derivatives.

4-62; 106-186;
(Givaudan data).

## 1695: HOMOVANILLIN

*4*-Oxy-*3*-methoxy phenylacetaldehyde.



$C_9H_{10}O_3$ = 166.18

White prismatic or leafy crystals. M.P. 51° C.
B.P. near 300° C.

Slightly soluble in water, somewhat soluble in hot water, soluble in alcohol and oils.

Floral Vanilla-like odor, sweeter and more delicate than the odor of Vanillin.

This comparatively rare material has been suggested for use in perfumes and flavors as a modifier for Vanillin/Ethylvanillin and other members of the Vanillin family. Probably on account of its higher cost of production, it has not become as popular as one should expect, considering the fact that it is more "Vanilla-like" than Vanillin, although overall weaker in effect. It has the same disadvantages from a chemical point of view, plus an added drawback in the poor stability under mildly alkaline and mildly acid conditions. It will resinify and become almost odorless under such conditions.

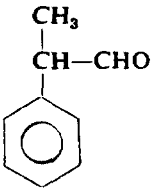
For these reasons it may also be evident that this material is not very suitable for flavor use, except in neutral Vanilla flavorings for Ice cream etc.

Prod.: (several methods, e. g.): from Eugenol in Ethylacetate solution by treatment with Ozone.

5-137; 7-207; 86-61; 95-146; 96-138;

## 1696: HYDRATROPALDEHYDE

Hydratropic aldehyde.
*alpha*-Methyl phenylacetaldehyde.
*alpha*-Phenyl propionaldehyde.
*2*-Phenylpropanal.
Hyacinthal.
Sylvanal.
*alpha*-Methyl tolualdehyde.
Ecorsal.
Vert de fleurs.
- and many other trade names.



$C_9H_{10}O$ = 134.18

Colorless liquid. Sp.Gr. 1.01. B.P. 204° C.

Almost insoluble in water, soluble in alcohol and oils.

Very powerful and penetrating, green-earthy, foliage-like odor in extreme dilution becoming quite floral, Lilac-Hyacinth-like and slightly fruity. Although it equals Phenylacetaldehyde in olfactory power, it is pleasantly free from the stinging pungency of the latter.

At dilutions below 1 ppm, the taste is rather sweet-earthy-green and somewhat fruity, depending upon accompanying acidity.

This aldehyde is frequently used in floral perfumes, first of all in Hyacinth, where it – in the opinion of many perfumers – outperforms Phenylacetaldehyde. It is furthermore much more stable that that Aldehyde, and does not tend to polymerize under normal use conditions. This aldehyde is also used in Rose, Narcisse, Lilac, Tulip and in many exotic floral types, as well as in certain non-floral fragrances.

Hydratrop aldehyde is used in flavor compositions for imitation Apricot, Almond, Cherry, Peach, Blackcurrent, Plum, Watercress, and in various Berry and Rose-floral complexes.

The concentration is normally mere traces, equivalent to about 0.3 to 1.0 ppm in the finished product.

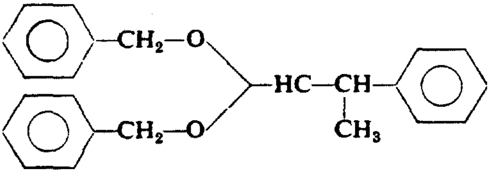
G.R.A.S. F.E.M.A. No.2886.

Prod.:

1) From Acetophenone and Ethyl chloroacetate via Phenylmethylglycidic acid.
2) By rearrangement of *2*-Phenylpropane-*1,2*-diol.
3) By reduction of Methyl phenyl acetylchloride.

4-63; 34-582; 68-528; 77-204; 86-61; 103-259; 106-187; 156-296;

## 1697: HYDRATROPALDEHYDE DIBENZYLACETAL



$C_{23}H_{24}O_2$ = 332.45

Colorless viscous liquid. Sp.Gr. 1.07.
B.P. over 300° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-earthy, somewhat nut-like and floral odor, reminiscent of Hawthorne and Hyacinth, but much milder and more tenacious than the Aldehyde.

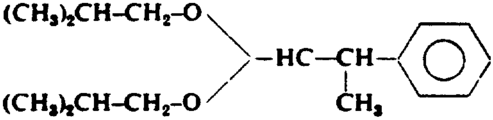
This Acetal has been suggested for use as a modifier for the Aldehyde or for some of the more common Acetals of the Aldehyde.

However, its odor does not seem to offer any particularly interesting notes or effects other than those obtainable with the Aldehyde and/or with the common Acetals.

Prod.: by condensation of Hydratropaldehyde with Benzyl alcohol.

33-158; 37-512;

## 1698: HYDRATROPALDEHYDE DI-iso-BUTYLACETAL



$C_{17}H_{28}O_2 = 264.41$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

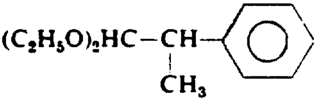
Sweet-earthy and nut-like odor resembling that of Coumarin, and with good tenacity. This Acetal is one of the least floral ones of the series, and its field of application is rather small.

It is rarely offered commercially, and the author is inclined to believe that this Acetal will become obsolete within some years.

Prod.: by condensation of Hydratropaldehyde and *iso*-Butanol.

28-555;

## 1699: HYDRATROPALDEHYDE DIETHYLACETAL



$C_{13}H_{20}O_2 = 208.30$

Colorless liquid. Sp.Gr. 0.93.

Insoluble in water, soluble in alcohol and oils.

Peculiar earthy-floral, musty-green odor. Some observers find a Peach-like note in this odor, but the author has not been able to personally underwrite this.

Although quite different from the Aldehyde itself, this Acetal has not achieved much interest, not nearly as much as the Dimethyl acetal. It does not have the typical "Champignon"-odor of the Dimethyl acetal, and the overall impression one gets is that of damp greenness with a trace of floral notes, but not reminiscent of any distinct natural material.

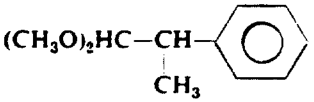
Prod.: by condensation of Hydratropaldehyde with Ethyl alcohol, usually supported by 1 to 1½% dry Hydrogen chloride to remove condensation water.

It can also be produced from the Aldehyde via Ethyl orthoformate reaction.

86-61; 86-115;

## 1700: HYDRATROPALDEHYDE DIMETHYLACETAL

"Lilanthal".
*2*-Phenylpropionaldehyde dimethylacetal.
*1,1*-Dimethoxy-*2*-phenylpropane.



$C_{11}H_{16}O_2 = 180.25$

Colorless liquid. Sp.Gr. 1.00.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, earthy, warm-spicy and green, deep-fruity odor, reminiscent of Walnut, Mushroom (Champignon) with a slightly floral-fruity undertone.

Warm-earthy, distinctly mushroomy taste in dilutions below 5 ppm. Higher concentrations are mostly nut-like, spicy or sharp.

This is the most important Acetal of Hydratropaldehyde. It finds use in perfume compositions for Lilac, Lily, Kewda (Pandanus) and in many other florals where green notes are important. Also for certain non-floral fragrances. It blends excellently with Coumarin and Nonanolide, with Amylsalicylate and Borneol, Rosemary and many dry-woody notes, etc. It gives interesting effects where Eugenol is present, and may often make Phenylacetic acid smell more attractive and pleasant.

The Acetal is also used in many types of flavor composition: Berry complexes, floral bases, Rose flavor, fruit complexes, imitation Honey, Nut and Spice, and particularly in Mushroom flavor. Concentration is usually very low, equivalent to 0.2 to 5 ppm in the finished product.

Hydratropaldehyde dimethylacetal gives interesting effects in Raspberry flavor in that it may reproduce the "nutty" aroma of the seeds (pits) of Raspberry, a flavor fraction necessary to complete the picture of natural Raspberry preserves, although not so necessary in juice.

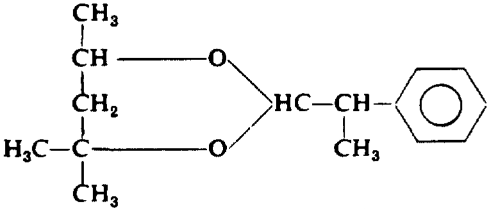
Prod.: by condensation of Hydratropaldehyde with Methanol, using dry Hydrogen chloride gas as condensing agent.

G.R.A.S. F.E.M.A. No.2888.

33-158; 77-209; 103-286; 106-188;

## 1701: HYDRATROPALDEHYDE-2,4-DIOXY-4-METHYLPENTANE ACETAL

*2-alpha*-Phenylethyl-*4,4,6*-trimethyl-*1,3*-dioxane.



$C_{15}H_{22}O_2 = 234.34$

Colorless oily liquid. B.P. 244° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, but relatively soft, green-herbal, earthy-green odor, reminiscent of Reseda (Mignonette).

A very large number of Acetals from Hydratropaldehyde have been prepared in the late 1930's and 1940's. Among the cyclic Acetals (using Glycols as the alcohol-portion in the condensation) probably the most interesting materials were found.

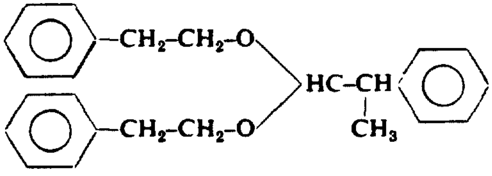
The subject cyclic Acetal is used in perfume compositions to introduce the earthy, almost root-like greenness which is often symbolized in the name Mignonette, a fragrance type which is created by the perfumer and not obtained from Nature. Reseda (Mignonette) is often combined with Roses in flower arrangements, and the two fragrances can also be combined in perfume formulations describing both. Very few materials describe the odor of Mignonette, and the subject Acetal is one such material.

It blends excellently with Phenylethylalcohol and many carbinols, with Linalool and substituted Linalools, etc. and with Vetiver, Patchouli and the Eugenols.

Prod.: by condensation of Hydratropaldehyde with *2*-Methylpentane *2,4*-diol (a chemical obtained in the Acetone reduction process). Mineral acid is used as condensing agent.

31-73;

## 1702: HYDRATROPALDEHYDE DIPHENYLETHYL ACETAL



$C_{25}H_{28}O_2 = 360.55$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Soft floral, deep-green and very tenacious odor with some resemblance to Rose foliage or Rose calice in a bouquet of Roses.

This Acetal, rarely offered under its proper chemical name, finds some use in perfumery as a modifier in variations of Rose bases, Rose fragrances, Oriental and woody odors, etc.

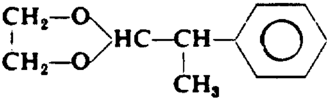
It blends well with the "rose alcohols" and with Cinnamic alcohol, the Eugenols, Sandalwood and Patchouli, etc. It tends to prolong the green notes already created by other components, usually more volatile, and thus acts in the "step-by-step" fixation (la fixation gradée).

Prod.: by condensation of Hydratropaldehyde with Phenylethylalcohol.

34-581;

## 1703: HYDRATROPALDEHYDE ETHYLENEGLYCOLACETAL

"Champignal".
"Foretine".
*2-(alpha*-Methylbenzyl)-dioxolane.
*2-(alpha*-Phenethyl)-*1,3*-dioxolane.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very earthy, sweet-green or musty, but delicate odor resembling that of Mushroom (Champignon).

Slightly bitter, Mushroom-like, but not exactly pleasant taste.

This Acetal is one of the most commonly used of the cyclic Acetals of Hydratropaldehyde. In spite of its very peculiar odor, it finds application in a great variety of fragrances and – because of its lack of sweetness – not much in flavor compositions.

Wherever such florals are desired which may have a forest-like odor nuance, or any connection with forest-odors, this Acetal may be useful. Muguet, noted for delicately fresh-humid forest-mossy background, or Gardenia with its dark-green foliage and Nut-like sweet-floral undertones, etc., may well benefit from the effects of this Acetal. Chypre, Fougère and other Oakmoss-carrying fragrances can achieve intriguing nuances with this material, and woody bases can be modified into new types.

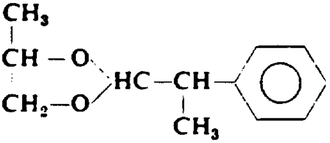
Coumarin and its derivatives are good secondary fixatives, and Opopanax is often a very interesting companion to this Acetal.

Prod.: by condensation of Hydratropaldehyde with Ethylene glycol.

4-30; 4-53; 4-275; 31-73; 77-209; 84-1; 50-359;

## 1704: HYDRATROPALDEHYDE PROPYLENEGLYCOLACETAL

*2-(alpha*-Methylbenzyl)-*5*-methyl-*1,3*-dioxolane.



$C_{12}H_{16}O_2 = 192.26$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-earthy, Mushroom-like odor with slightly fruity-green undertones and moderate tenacity.

Earthy-fungus-like taste, but slightly bitter and not quite pleasant.

This acetal has been suggested for use in perfume compositions as a modifier for the Ethyleneglycol-acetal (see previous monograph), but it has not achieved quite the same popularity.

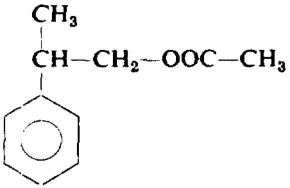
It resembles the Ethylene glycol acetal very much in odor type and taste, but it is not as typically Mushroom-like as that Acetal.

Prod.: by condensation of Hydratropaldehyde with Propyleneglycol.

101-2;

## 1705: HYDRATROPYL ACETATE

*alpha*-Phenylpropyl acetate.
*alpha*-Methyl phenyl acetate.
*2*-Phenyl propylacetate.



$C_{11}H_{14}O_2$ = 178.23

Colorless liquid. Sp.Gr. 1.07.

Almost insoluble in water, soluble in alcohol, miscible with oils. Fairly soluble in Propylene glycol.

Fresh-floral, powerful and fruity-green, slightly earthy-green odor more delicate than Phenylethylacetate, not as rosy, more Hyacinth-Lilac-like. Inspite of its power, or rather "lift", its effect is almost a delicate one, enabling the perfumer to use 2-4-6% of this ester in floral bases where green or green-earthy or spicy notes are already composed or called for.

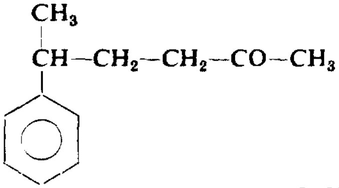
The ester finds use in Hyacinth, Lilac, Ylang-Ylang, Narcisse, etc. as well as in Oriental blends, where it gives pleasant combinations with the Phenylacetates or Cinnamates, particularly soothing on Methyl-cinnamate.

Prod.: by direct esterification of Hydratropyl alcohol with Acetic acid under azeotropic conditions, or with Acetic anhydride.

4-63; 34-583; 86-61;
(sample: I.F.F.).

## 1706: HYDRATROPYL ACETONE

*alpha*-Phenylpropyl methylketone.
*alpha*-Phenylpropyl propanone.
*5*-Methyl-*5*-phenylpentanone.
*5*-Phenylhexan-*2*-one.



$C_{12}H_{16}O$ = 176.26

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

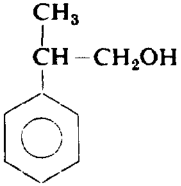
Sweet and honey-like, slightly fruity odor of considerable diffusive power and moderate tenacity.

This ketone finds some use in perfumery as a component of sweet-floral or honey-like bases. It blends excellently with the Phenylacetates, Heliotropine, the Ionones, Hydroxycitronellal and many Cinnamates and Phenylpropionates. It gives interesting effects with Valerates of aromatic alcohols (Benzyl-, Phenylethyl-, etc.), and with Phenylglycidic esters.

Prod.: from Hydratropaldehyde by condensation with Acetone followed by hydrogenation of the condensation product.

## 1707: HYDRATROPYL ALCOHOL

Hydratropic alcohol.
*alpha*-Methyl phenylethyl alcohol.
*2*-Phenyl propan-*1*-ol.
*alpha*-Phenylpropyl alcohol.
Note: This material is sometimes called:
*beta*-Phenylpropyl alcohol.



$C_9H_{12}O$ = 136.20

Colorless liquid. B.P. 219° C. Sp.Gr. 1.02.

Slightly soluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Sweet-floral, but rather heavy odor of Lilac-Hyacinth type. Commercial products are rarely of high olfactory purity and may show variable amounts of harsh or "gassy" or Acetophenone-like topnotes which partly or wholly ruin the overall odor impression. This may also be the reason why perfumers generally do not even carry this material on their shelf – a simple objection to the material as it was first presented to them. Truly, an olfactorily pure grade of Hydratropyl alcohol shows quite interesting odor and should give the creative perfumer many good ideas.

It blends well with the "rose alcohols", with Eugenols and woody odors, with Oakmoss products and Vetiver, etc. With suitable blending in Cinnamic alcohol and derivatives, it may form background for Hyacinth and other floral bases.

This alcohol is occasionally used in flavor compositions, usually as a trace component in Berry, Melon, Honey and Nut compositions, or in rare floral flavor types. Its taste is rather heavy-sweet, woody-floral, but pleasant in concentrations below 20 ppm. Common use level is 0.5 to 1.5 ppm.

G.R.A.S. F.E.M.A. No.2732.

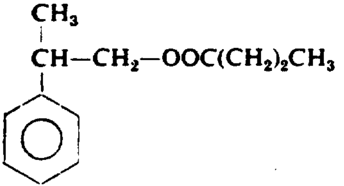
Prod.: (many methods), e. g.: by hydration of *alpha*-Methyl styrene.

4-63; 34-582; 68-501; 86-61;

## 1708: HYDRATROPYL BUTYRATE

*beta*-Methyl phenylethyl butyrate (F.E.M.A. name).

2-Phenylpropyl-*n*-butyrate.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Fruity-floral, and slightly spicy odor with faintly woody undertones. Overall rather heavy, but pleasant.

Heavy-fruity, slightly spicy taste in dilutions below 5 ppm. Higher concentrations tend to give a "perfumey" taste.

This ester, rarely offered commercially, is sometimes used in floral or woody-floral perfume compositions as a modifier or as a "new" note.

It finds also some use in flavor compositions of the heavy-fruity type, e. g. Peach and Mango, usually in concentrations as low as 1 to 2 ppm in the finished product.

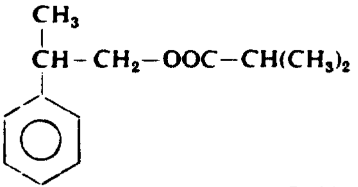
Prod.: by direct esterification of Hydratropyl alcohol with *n*-Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2891.

See also monograph No. 1165.

## 1709: HYDRATROPYL-iso-BUTYRATE

2-Phenylpropyl-*iso*-butyrate.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Fruity-woody, very sweet and somewhat heavy, but overall pleasant odor.

Fruity and sweet taste, reminiscent of Prune and Plum preserve, heavy but in a pleasant and rather natural way.

This ester is generally preferred over the *n*-Butyrate for being less heavy and somewhat fresher in its overall performance.

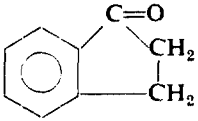
The ester finds very little use in perfumery, but it is used in flavor compositions where heavy-fruity notes are desirable, e. g. imitation fruit preserve, Plum, Prune, Blackcurrant, etc. Concentration is normally about 5 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2892.

Prod.: by direct esterification of Hydratropyl alcohol with *iso*-Butyric acid under azeotropic conditions.

## 1710: alpha-HYDRINDONE

*1*-Indanone.
*1*-Ketoindane.



$C_9H_8O$ = 132.16

Rhombic colorless crystal needles, melting at 41° C. B.P. 244° C. Sp.Gr. 1.10 (liquid).

Slightly soluble in water, soluble in alcohol, miscible with oils.

Rather weak, woody and somewhat medicinal odor with an incense-like undertone.

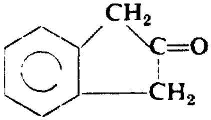
It may be because of its remote resemblance to incense, that this odor has caught any interest at all. Apart from that, there is not much to be said, except that the material could be of academic interest for olfactory studies. The author believes that subject ketone is rarely, if ever, used in perfumes or flavors.

Prod.: by cyclization of *beta*-Phenylpropionyl chloride in Benzene.

4-63; 26-576; 68-1265; 160-1050; B-VII-360;

## 1711: beta-HYDRINDONE

*2*-Indanone.
*2*-Ketoindane.



$C_9H_8O$ = 132.16

Colorless needle-like crystals. M.P. 61° C. B.P. 227° C. (decomposes). Sp.Gr. 1.07 (liquid).

Insoluble in water, soluble in alcohol and oils.

Rather weak, sweet-medicinal, moderately tenacious odor with a faint resemblance to notes in Civet. Overall woody-hydrocarbon-like.

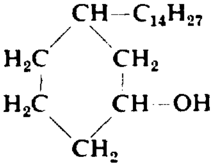
This material is mentioned mainly for the completion and illustration of the series in which *alpha*- and *beta*-Hydrindone have been emphasized as having potential interest to the perfume industry. It is the author's impression that the two materials are not used in perfumes or flavors.

Prod.: (several methods) e. g. by boiling Indene oxide with diluted Sulfuric acid.

68-1266; 160-1050;

## 1712: HYDROCARDANOL

Dihydrocardanol.
NOTE: see also monograph: Cardanyl benzoate.



$C_{20}H_{38}O$ = 294.52

Colorless or very pale straw-colored viscous liquid.

Insoluble in water, soluble in alcohol, miscible with oils.

Very faint, dry-woody, slightly camphoraceous odor of considerable tenacity.

This *meta*-substituted Cyclohexanol has been suggested for use in perfume compositions as a fixative with very limited odor contribution.

The author is of the impression that this chemical has been produced in the late 1930's as a result of considerable research on the subject of utilization of by-products from Cashew-nut production. The edible "nut" (the kernel) is surrounded by a shell (mesocarp) in which a slow-drying (fixed) oil is contained. The oil contains Cardol, Cardanol and other components. Cardol is particularly hazardous as a vesicant and irritant, and must be quantitatively separated from the kernels intended for food use.

The amount of shells in proportion to the kernels is enormous, and it has been a problem to find good use for the shell oil. It has been used in varnishes, laundry-marking ink, as a proteolytic solvent to remove corns and callouses, as a fabric dye, etc. but most of these uses are obsolete with superior or cheaper products available. The swollen receptacle is known as "Cashew-Apple" and its Apple-tasting pulp is a local delicacy in India and the West Indies. But the vesicant oil remains a problem. The chief component, Cardanol has been isolated and investigated. Hydrogenation yields the so-called Hydrocardanol (at one time called Carhydranol, this name now used for a different alcohol).

Hydrocardanol is a non-irritating oil, and it does not resinify or "dry" so easily. But its use in perfumery is, in the author's opinion, obsolete, and was never important.

It is worthwhile remembering that the edible nut, Cashew, amounts to only 2 to 4% of the total "fruit" (including the "Apple") by weight, and that full use of the remaining fruit parts is necessary for the economy of Cashew-kernel production.

Prod.: by hydrogenation of Cardanol, isolated from Cashew-shells.

31-25;

## 1713: HYDROCYANIC ACID

"Prussic acid".
Hydrogen cyanide.
Formonitrile.

$H-C\equiv N$

$HCN = 27.03$

Colorless mobile liquid, boiling at 26° C. Colorless gas at temperatures above 27° C. Sp.Gr. 0.69 (liquid).

The gas is slightly lighter than air.

Miscible with water and alcohol, soluble in most oils.

Sweet odor reminiscent of mashed Bitter Almonds, but more woody and delicate.

Note: Extremely poisonous. Lethal dose for human beings is about 0.05 grams or the equivalent of exposure to 300 ppm in the air for 1 to 2 Minutes.

This material is mentioned because it forms part of an essential oil which is used extensively in flavorings, although it is commonly specified that Bitter Almond oil should be free from this acid (F.F.P.A.).

The acid occurs together with Benzaldehyde in the enzymatic hydrolysis of a glycoside in the Bitter Almond kernel in the presence of water. Bitter Almonds produce Hydrocyanic acid upon chewing. 10 or more almonds present a hazardous dose to the human system.

The acid is present in crude Bitter Almond oil at the rate of 2 to 4%. The acid is usually removed by mild alkali washing and rectification. Accidental intake of 10 drops of unrectified Bitter Almond oil can cause death to an adult human being. Yet, the acid still finds use in medicine in low-concentration aqueous solution.

It is interesting to note that the two decomposition products from the Bitter Almond glycoside, Benzaldehyde and Hydrogen cyanide, have similar odors, yet are chemically very different.

On the other hand, Nitriles are often found to have odors similar to those of the corresponding Aldehyde. The subject material forms an obvious exeption from the "rule".

Prod.: by catalytic oxidation of Ammonia plus Methane gas.

26-578; 77-212; 100-534; 104-52; 160-1046; B-II-29;
see also monograph: Mandelonitrile.

## 1714: HYDROGEN SULFIDE

"Hydrosulfuric acid" (old name).

$H_2S = 34.08$

Colorless gas. Specific gravity (air = 1.00) 1.19.

Soluble in water, alcohol, glycerin and in some oils.

Very unpleasant, chokingly repulsive odor, often described as reminiscent of "rotten eggs" or "decaying seaweed", etc. both of which products are literally oozing out Hydrogen sulfide in the state described.

The odor is perceptible at concentrations of about 0.002 milligrams per liter of air. This is approximately equivalent to 1.3 ppm in gas phase.

Note: Hydrogen sulfide is extremely poisonous and is not to be used in flavors. It is also very explosive in mixtures with air.

This material is mentioned in the present work mainly because it occurs in many freshly distilled essential oils, particularly those distilled from fruits of plants of the Umbellifer order, such as Caraway, Fennel, Anise, Angelica, Cumin, etc. and also in certain other oils: Black Pepper, Clove bud, etc.

It is furthermore found in oils distilled with poor grade water (Eucalyptus, Petitgrain, Bois de Rose, etc.).

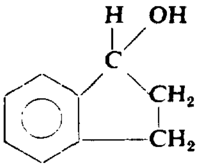
Although it might in some cases contribute to the peculiar topnote of an essential oil, it is common practice to remove Hydrogen sulfide prior to use of essential oils in perfumery. The cleaning process may be a simple "airing", bubbling with Nitrogen or $CO_2$, gentle heating or washing.

Prod.: by reacting Sulfur with Hydrogen in vapor phase.

26-256; 100-536; 160-582;

## 1715: HYDROINDOL

Sometimes called Hydrindole.
Indan-*1*-ol.
*1*-Hydroxyindane.
*2*-,*4*- and *5*-Hydroxyindanes are known.



$C_9H_{10}O = 134.18$

Colorless or white crystals. M.P. 41° C. and 53° C. (the material is dimorphous).

Almost insoluble in water, soluble in alcohol, soluble in some oils.

Peculiar woody-smokey odor, reminiscent of the Cresols, but sweeter and milder, more smokey, less medicinal.

Has been suggested for use in perfume compositions, but there seems to have been little interest in this material. Indane derivatives have later found use as Musk odorants, but the lower members, such as the subject alcohol, lacks characteristic and attractive notes and does not fill in an urgent need for the perfumer.

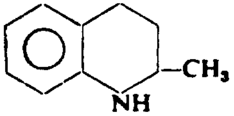
Prod.: by hydrolysis of *1*-Chloroindane with Potassium carbonate at 60° C.

*4*-Hydroxyindane can be isolated from coal tar.

4-63; 68-1264;

## 1716: HYDROQUINALDINE

Tetrahydro-*2*-methylquinoline.
*2*-Methyl tetrahydroquinoline.
*alpha*-Methyl tetrahydroquinoline.



$C_{10}H_{13}N = 147.22$

Pale straw-colored or pale-amber colored oily liquid, becoming darker upon age or exposure to air or daylight.

Very slightly soluble in water, soluble in alcohol, miscible with most oils.

Powerful and rich, sweet-floral odor with resemblance to Lilac. Slightly animal undertone and good tenacity.

This Amine is used in perfumery as a modifier for the conventional Lilac materials (Terpineol-Linalool-etc.), and in general as a floralizer in heavy or very deep-sweet florals where slightly animal notes are tolerated or desirable.

It may in such cases partly replace Terpineol to introduce more depth and less piney-woody tones.

Several isomers of the subject material are commonly used in perfumery, see:

Tetrahydro-*para*-methylquinoline, and the unsaturated Methylquinolines (5 isomers).

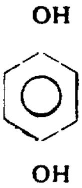
Prod.: (many methods):

1) from *ortho*-Toluidine and Acrolein with Stannic chloride (or with Glycerin plus Sulfuric acid) in the so-called Skraup-reaction.
2) by reduction of Quinaldine (obtainable from coal tar) with Hydrogen and a catalyst.
3) from Aniline plus Acetaldehyde via Quinaldine.

3-57; 4-63; 34-583; 86-99; 31-191; 37-939;

## 1717: HYDROQUINONE

*para*-Dihydroxy benzene.
Hydroquinol.
Quinol.
Tecquinol.
*1,4*-Dihydroxybenzene.



$C_6H_6O_2 = 110.11$

White crystals. M.P. 172° C. B.P. 287° C.

7% soluble in water, soluble in alcohol. Soluble in some, but not all, oils.

The pure chemical is virtually odorless. Commercial grades may carry a faintly phenolic odor.

Its taste is sweet in concentrations near 50 ppm, but the sweetness is accompanied by an astringent mouthfeel at higher concentrations of the material.

Although Hydroquinone as such is not considered a perfume or flavor chemical, it is included in this work for several reasons:

Hydroquinone has been, and still is, used as a food antioxidant. It is very easily oxidized, particularly in presence of alkali.

Hydroquinone is listed by the American F.E.M.A. as G.R.A.S. It is interesting to note that the *1,3*-isomer, Resorcinol, is approved by the U.S. Federal Register for use as a food additive, while the third isomer, Catechol (the *1,2*-isomer) is not listed by any of the two authorities.

Newer and much more effective antioxidants have been developed, some are derivatives of Hydroquinone. It is most conceivable that Hydroquinone is losing its importance as a food antioxidant.

Prod.:

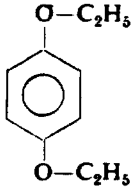
1) from *para*-Chlorophenol by heating with Sodium hydroxide solution to 200° C.

2) from *para*-Dichlorobenzene by similar treatment.
3) from *para*-Hydroxybenzaldehyde by oxidation with Hydrogen peroxide.
– and many other methods.

26-506; 68-475; 100-537; 159-400; 159-497; B-VI-836;

## 1718: HYDROQUINONE DIETHYLETHER

*para*-Diethoxybenzene.
Quinol diethylether.



$C_{10}H_{14}O_2 = 166.22$

White crystal leaves, melting at 72° C.
B.P. 245° C.

Volatile with steam. Insoluble in water, soluble in alcohol, miscible with most oils. Poorly soluble in Propylene glycol.

Anisic-minty odor of considerable tenacity. The sweetness is somewhat impaired by the peculiar "mintiness" or "lack of warmth", a characteristic which makes this ether one of the least interesting of the series (there are at least 5 members of more or less interest to the perfume and flavor industry).

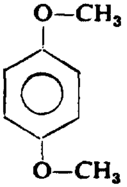
This ether has been suggested for use in perfume compositions as a modifier for Coumarin and Acetanisole, etc. It will contribute a fair amount of fixation and a novel type of sweetness, but it lacks the herbaceous warmth of the materials which it is supposed to replace or modify.

Prod.: by Ethylation of Hydroquinone with Diethylsulfate in weak aqueous alkali.

26-494; 31-147; 68-476; 90-385; B-VI-844;

## 1719: HYDROQUINONE DIMETHYLETHER

*para*-Dimethoxybenzene.
Quinol dimethylether.
Dimethyl hydroquinone (Commercial name, chemically incorrect).
"Hazeltone".
"Noisette".
"Tonkaine".



$C_8H_{10}O_2 = 138.17$

White crystals, leaves or crystalline mass, melting at 56° C. Sp.Gr. 1.04 (liquid).
B.P. 213° C.

Volatile with steam, sublimes when heated dry. Slightly soluble in water, fairly soluble in alcohol, soluble in most perfume and flavor materials.

Warm-herbaceous and Nut-like, tobacco-like odor of considerable power and good tenacity (in spite of low boiling point).

Intensely sweet, Nut-like, warm taste in dilutions below 5 ppm. It creates synergistic effects with many conventional sweeteners, Coumarin, Vanillin, Heliotropin, etc.

Widely used in perfume compositions, although generally at very low concentration (perceptible effects well below 1 % in the perfume oil). It forms part of the herbaceous theme in many New Mown Hay, Tobacco-, Hyacinth, Hawthorne, Carnation, Melilotus, etc., and supports floral notes in Gardenia, Honeysuckle, Mimosa, Hyacinth and many others. It gives interesting effects in Pine Needle fragrances, in Ambre bases and, in general, as an additive to Coumarin or Nonanolide.

This ether finds also considerable use in flavor compositions, although only traces are used in Raspberry, Fruit complexes, Nut flavor imitations, Hazelnut, Vanilla, Root Beer, etc. Its tenacity makes it a preferred item in flavors for baked goods and wafers, and it is often used as a fortifier for Vanilla flavors for ice cream, etc. Concentration amounts to a few ppm in the finished products.

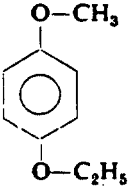
G.R.A.S. F.E.M.A. No.2386.

Prod.: by Methylation of Hydroquinone with Dimethylsulfate in weak aqueous alkaline solution.

4-45; 4-63; 26-512; 68-476; 86-47; 86-61; 90-386; 103-219; 103-306; 106-138; B-VI-843;

## 1720: HYDROQUNINONE METHYL ETHYL ETHER

*1*-Methoxy-*4*-ethoxybenzene.
Quinol methylethyl ether.



$C_8H_{12}O_2 = 152.20$

White or colorless crystal leaves or crystalline mass, melting at 39° C. Poorly soluble in alcohol, soluble in perfume and flavor materials. Insoluble in water.

Sweet and moderately warm-herbaceous odor, reminiscent at the same time of Anise and Fennel.

Sweet-herbaceous but slightly burning taste in dilutions near 10 ppm. Lower concentrations taste sweet and slightly spicy.

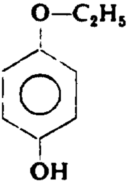
This ether has been suggested for use in perfume formulations where Anise-Fennel odors are called for. It has been used in the reconstruction of Fennel oil, but that oil is not in very strong demand. The particular odor type is not often wanted in perfumery, and since Anethole or technical grade Anethole are available at very low cost, it is most conceivable that this – and similar – material will become obsolete.

Prod.:
1) by Ethylation of Hydroquinone monomethylether.
2) by Methylation of Hydroquinone monoethylether.

31-147; 34-679; 68-476;

## 1721: HYDROQUINONE MONOETHYLETHER

*1*-Ethoxy-*4*-hydroxybenzene.
*para*-Hydroxyphenethol.
*para*-Ethoxyphenol.
Quinol monoethylether.



$C_8H_{10}O_2 = 138.17$

White or colorless crystal leaves. M.P. 66° C. B.P. 247° C.

Slightly soluble in cold water, soluble in hot water, alcohol and oils. Fairly soluble in Propylene glycol.

Sweet-herbaceous odor, reminiscent of Anise and Fennel, but not as sweet as Hydroquinone methylethylether.

Slightly bitter-metallic taste, through which the sweetness is barely perceptible. Overall not a pleasant taste.

This material is rarely used in perfumes as an odorant, but it is included in this work partly for the reason of completing the series of Hydroquinone ethers, partly because this material is used in a number of perfume materials as an antioxidant or stabilizer to retard the deteriorating effect from contact with air.

As an antioxidant, it does not compete well with the more modern Butylated hydroxytoluene or Butylated hydroxyanisole, nor with certain Gallates and certain more complicated chemicals.

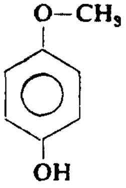
It has advantage of better solubility in certain perfume materials and its odor is compatible with many such materials. Like most other antioxidants, its effect lies in the fact that it absorbs oxygen faster than the product which it protects, in other words, it "steals" the oxygen away from the perfume material (or composition). Its action is therefore limited and it can only prolong the life of the acceptable fragrance, rarely forever preserve it.

Prod.: by regulated (Mono)-ethylation of Hydroquinone with Diethylsulfate in weak aqueous alkaline solution.

26-538; 31-147; 34-679; 61-53; 90-385; 96-98; B-VI-843;

## 1722: HYDROQUINONE MONOMETHYLETHER

*1*-Methoxy-*4*-hydroxybenzene.
*para*-Hydroxyanisole.
*para*-Methoxyphenol.
Quinol monomethylether.
"Monomethyl hydroquinone".



$C_7H_8O_2 = 124.14$

Colorless or white, leafy crystals. M.P. 56° C.
B.P. 243° C.

Slightly soluble in water, soluble in alcohol, miscible with oils.

Sweet, "aromatic" odor, reminiscent of Anisole, but much weaker and milder, not harsh. Chemically pure Hydroquinone monomethylether has very little odor.

For completion of the series of Hydroquinone ethers, this material is briefly mentioned. It is also used as an antioxidant – see previous monograph on the Monoethylether.

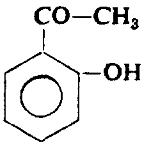
To the author's knowledge, there is no significant use of this material in perfumes or flavors beyond that as an antioxidant.

Prod.: by regulated (Mono)methylation of Hydroquinone with Dimethylsulfate in weak aqueous alkaline solution.

26-596; 68-476; B-VI-843;

## 1723: ortho-HYDROXY ACETOPHENONE

*2*-Hydroxy acetylbenzene.
*2*-Acetyl phenol.



$C_8H_8O_2 = 136.15$

Almost colorless oily liquid. Sp.Gr. 1.13.
Solidifies in the cold, and melts again at 5° C.
B.P. 220° C.

Slightly soluble in water, soluble in alcohol and oils.

Sweet and rather heavy-floral, also somewhat herbaceous odor, reminiscent of New Mown Hay or Hawthorne in higher concentration, almost Mimosa-like in extreme dilution.

The odor has sometimes been described as resembling that of the flowers of the "Snowdrop-tree", but unfortunately this tree is not common outside of Virginia and the Carolinas in the Eastern United States, so it is of little value to everybody else to use those flowers for comparison.

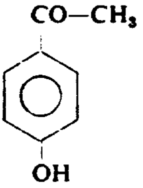
This simple, but relatively rare chemical has been suggested for use in perfume compositions as a modifier for Coumarin, Methylacetophenone, Acetanisole, etc. as a powerful floral, heavy background note in Acacia, Mimosa, Wallflower, and in various floral bouquets.

Prod.: from Phenylacetate by heating with Aluminium chloride. A mixture of *ortho-* and *para*-hydroxyacetophenone is formed, and the ratio can be controlled by heat and other conditions.

26-578; 36-1255; 68-431; 103-275; B-VIII-85;

## 1724: para-HYDROXY ACETOPHENONE

4-Hydroxy acetylbenzene.
4-Acetyl phenol.



$C_8H_8O_2 = 136.15$

Colorless needles melting at 109° C.
Sp.Gr. 1.11 (liquid). B.P. 286° C.

1 % soluble in water, soluble in alcohol and oils.

Heavy-floral, somewhat herbaceous or woody-haylike odor of considerable tenacity. Slightly more floral than the *ortho*-isomer (see previous monograph) also more tenacious and overall somewhat more pleasant. Yet, they both could be classified as "harsh" odor types with little similarity to natural odors.

This ketone has been suggested for use in perfume compositions as a modifier for the more conventional derivatives of Acetophenone, etc. mainly in heavy-floral or woody-floral fragrances where power and low cost are requested.

It does not have the power or sweetness of its Methylether (Acetanisole) and will probably never attain much popularity no matter how inexpensive it may become.

The author believes that these two phenolic ketones will become obsolete or at least will remain of very limited interest to the perfumer.

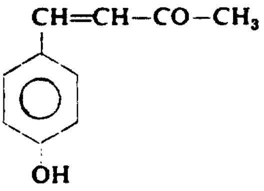
Prod.:

1) from Phenylacetate by heating with Aluminum chloride (see previous monograph).
2) from Phenol, Acetylchloride and Aluminum chloride by Friedel-Craft' reaction.

26-578; 68-431; B-VIII-87;

## 1725: para-HYDROXY BENZALACETONE

*para*-Hydroxy phenylbutenone.
*para*-Hydroxy benzylidene acetone.



$C_{10}H_{10}O_2 = 162.19$

Exists in 2 modifications. Colorless or yellow needlelike crystals. M.P. 112° C.

Poorly soluble in water, soluble in alcohol, soluble in some perfume and flavor oils.

Herbaceous-sweet, somewhat dry odor. Overall rather mild and not very tenacious.

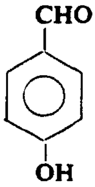
The author is not aware of this material being used in perfume compositions as such. It is an intermediate in the manufacture of the so-called "Raspberry ketone" another important natural component material, see *para*-Hydroxyphenylbutanone.

The subject ketone is used in flavor compositions, almost exclusively in imitation Tea flavor or in the reconditioning of Tea flavor.

Prod.: by condensation of *para*-Hydroxybenzaldehyde and Acetone and acidification of the reaction mixture (cold process).

90-542;

## 1726: para-HYDROXY BENZALDEHYDE



$C_7H_6O_2 = 122.13$

White powder or crystal needles.
M.P. 116° C. Sp.Gr. 1.13 (liquid). Sublimes when heated.

1.4% soluble in water, soluble in alcohol, but poorly soluble in most oils.

Very faint, sweet-woody-balsamic odor. Chemically pure aldehyde is virtually odorless.

The taste of this aldehyde is sweet with little or no other flavor impression. The sweetness is perceptible in aqueous solutions of less than 1% aldehyde.

Although in itself not a perfume material and hardly a flavor material, this aldehyde deserves mention because it is extremely important as an intermediate in the manufacture of many interesting perfume and flavor chemicals. It is also a breakdown product in Nature's Lignin decomposition, and therefore present, mostly in the shape of derivatives, in numerous natural products.

With Acetone it gives by condensation, followed by hydrogenation, one of the most interesting Raspberry flavor materials of many decades, see *para*-Hydroxyphenylbutanone.

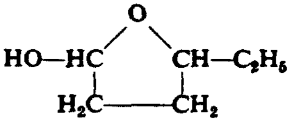
The subject aldehyde is produced by many ways, e. g.:

1) from Phenol in the manufacture of Salicylic aldehyde (which is the *ortho*-isomer).
2) from *para*-Aminobenzaldehyde by Diazo-reaction.
3) from Phenol and anhydrous Zinc cyanide in Benzene, followed by hydrolysis.

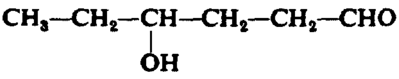
26-578; 68-744; 100-538; 160-828; B-VIII-64

## 1727: gamma-HYDROXY CAPROIC ALDEHYDE

*gamma*-Hydroxy-*n*-caproäldehyde.
*gamma*-Hydroxy-*n*-hexanal.
This chemical occurs mainly in the shape of a hydroxylactone-form:
(a cyclic semi-Acetal):



and to a lesser degree as:



$CH_3-CH_2-CH(OH)-CH_2-CH_2-CHO$

$C_6H_{12}O_2 = 116.16$

Colorless oily liquid. Sp.Gr. 1.00.
B.P. 191° C.

Refreshingly green-vegetable odor reminiscent of Cucumber, Watermelon (rind) and very young, undeveloped leaves. There is an almost citrusy freshness in this delicate greenness.

The aldehyde has been suggested for use in flavor compositions for imitation "fresh-fruit" and "fresh-vegetable" notes, particularly in Melon, Gooseberry, Apple, etc.

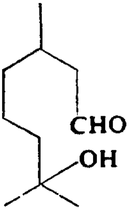
The aldehyde could undoubtedly find use in perfume compositions, but it is possible that interest is lacking due to the overwhelming number of "green" odorants that have appeared on the market during the past decade or so.

Prod.: from Allyl acetic acid.

66-706;

# 1728: HYDROXYCITRONELLAL

7-Hydroxy-*3*,*7*-dimethyloctan-*1*-al.
Oxydihydrocitronellal.
Citronellalhydrate.
Cyclosia base (Firmenich).
Laurine (Givaudan).
Hycelea – Laurinal – Storine – Centaflor – Majal – Cyclodor – Fixonal – Cyclia – Phixia – Anthosal – Hylea – Muguettine principe – Cyclalia – Lilyaldehyde – Fixol – Muguet synthetique – Tilleul – Cyclohydronal – and many other trade names.



$C_{10}H_{20}O_2 = 172.27$

Colorless oily or viscous liquid. Sp.Gr. 0.93. B.P. 241° C.

Very slightly soluble in water, soluble in alcohol and oils. Poorly soluble in mineral oil and Glycerin or Propylene glycol.

Sweet-floral, at first delicate and refreshingly mild, but often increasing in odor strength after short olfactory study. The floral notes are mild, light and resemble Lily of the Valley. The tenacity is good, and the odor diffusion increases significantly when the material is properly blended with lower boiling odorants or modifiers.

There is a marked difference in the topnote of this material from different suppliers. Only few manufacturers make a material with a truly uniform, delicately floral odor performance from the very first (initial) note to the terminal notes (dryout, dry-down-notes).

The odor will remain for days, weeks or even longer, but the material on a testing blotter is obviously exposed to air attack and polymerization. A good way – but a very strict one – to evaluate this aldehyde is in lukewarm water. It is sufficiently soluble that it will show water-insoluble impurities strongly enhanced on this test. A very fine grade of Hydroxycitronellal will have almost the same odor on this test as it has on a perfume blotter.

Hydroxycitronellal has a sweet-floral taste, but shows a bitter aftertaste at concentrations higher than 20 ppm, sometimes even much lower than that.

This aldehyde is one of the most frequently used floralizing perfume materials. Originally introduced as a "Muguet" material, it finds its way into almost every type of floral fragrance, and a great many nonfloral ones. Its concentration in perfumes may vary from about 1 % (which rarely gives effect unless supported by parallel materials) up to 30 or 40 % in straight floral types.

It is almost a "must" in Muguet (at certain price levels) and Peony, Lily, Sweet Pea, Narcisse, Lindenblossom, etc. and it had a monopoly on these types for more than 40 years during which period not one material appeared that could truly replace Hydroxycitronellal. And even after the appearance of one of several very good, perhaps superior – materials, the demand for Hydroxycitronellal kept increasing. Endless discussions about its possibly irritating effect on the human skin have hardly died out yet – but Hydroxycitronellal has now reached and by-passed the one-million-pounds per year mark in a volume class reserved for comparatively few perfume materials.

For soap perfumes it is customary to use a slightly more "rough" grade of this material. Power is often of paramount interest to the soap manufacturer when it comes to perfuming, and the very pure grade materials with delicate odors often fail to yield the desirable power in a soap.

High-grade Hydroxycitronellal is used sparingly in flavor compositions as a floralizer in many types of flavor: Berry complexes, Citrus, Violet, Cherry, etc. and in general, a discrete touch of floral note in a flavor tend to give impression of "richness" or "body" which are highly desirable virtues. In some cases, a complete Muguet base is added to a flavor – fruit, Mint, etc. – to lend this "rounding-off" effect. The amounts needed are mere traces.

Hydroxycitronellal enters these flavor types at the concentration equal to 0.3 to 15 ppm in the finished product.

Prod.: (many methods) e. g. from Myrcene, via Myrcene dihydrochloride to Dichloro dimethyloctene. This is converted to Chloro dihydrogeranyl acetate (and -neryl acetate) with Sodium Acetate in Benzene in presence of Triethylamine. The acetates are saponified with Calcium hydroxide to yield Hydroxycitronellol, from which the aldehyde is prepared by oxidation.

Older methods start from Citronellal via the Bisulfite which is hydrated to yield Hydroxycitronellal.

G.R.A.S. F.E.M.A. No.2583.

4-63; 7-179; 31-43; 34-806; 61-49; 85-69; 86-61; 106-189; 156-182; 5-99; 5-353;

## 1729: HYDROXYCITRONELLAL DI-iso-BUTYLACETAL

$C_9H_{18}CH(OCH_2{-}CH(CH_3)_2)_2OH$
(structure, - see Hydroxycitronellal)

$C_{18}H_{38}O_3 = 302.50$

Colorless oily liquid.

Very faint green-floral odor of considerable tenacity.

This is probably one of the least interesting Acetals of Hydroxycitronellal. Its lack of power and of distinctly different or unusual notes will probably put this material back into oblivion or at least on the research shelf. It has, in the author's opinion, no mission in the perfume laboratory.

Prod.: by condensation of Hydroxycitronellal and *iso*-Butanol.

4-64;

## 1730: HYDROXYCITRONELLAL DIETHYLACETAL

$C_9H_{18}CH(OC_2H_5)_2OH$

$C_{14}H_{30}O_3 = 246.39$

Colorless, slightly oily liquid. Sp.Gr. 0.92. B.P. approximately 260° C.

Almost insoluble in water, soluble in alcohol and oils.

This acetal seems to be of little or no interest to the perfumers, but it does find some application in flavor compositions.

It has a delicately green-floral taste and is not as bitter as the Aldehyde itself. Its odor is very mild, in fact, some observers find it practically odorless.

It is used in various fruit and Citrus flavors in very low concentration, equivalent to about 0.5 to 10 ppm in the finished product.

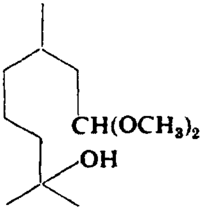
It is worthwhile noticing that this Acetal is used in flavors in which acid is used for additional fruit taste. Acetals, including this, tend to decompose under mildly acid conditions, and one would expect that Hydrocitronellal eventually appears in the flavor where the Acetal has been incorporated - once the flavor is used in the functional, acidified product.

G.R.A.S. F.E.M.A. No.2584.

Prod.: by condensation of Hydroxycitronellal with Ethanol, using dry Hydrochloric gas as condensing agent.

## 1731: HYDROXYCITRONELLAL DIMETHYLACETAL

*1,1*-Dimethoxy-*3*,7-dimethyloctan-7-ol.
Muguene.



$C_{12}H_{26}O_3 = 218.34$

Colorless, slightly oily liquid. Sp.Gr. 0.93. B.P. 252° C.

Almost insoluble in water, insoluble in Glycerin, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Very faint, green and fresh-floral odor of good tenacity. Some observers find this material to be practically odorless. It does produce a perceptible odor in combination with other odorants, particularly with lower boiling ingredients.

This Acetal finds use as a modifier for the Aldehyde – with very little effect – and in floral bases for powders, etc., where greater stability and tenacity are desired. The alledged greater stability in soap does not mean so much now, since soaps (and other cosmetic products) are made with better grade raw materials, and the hazard of decomposition of Hydroxycitronellal in soap greatly diminished. The use of the Acetal is therefore becoming a habit of the past, and the author believes that this Acetal will be confined to very few applications eventually.

It finds some use in flavor compositions for the same reasons as indicated under Hydroxycitronellal diethylacetal.

It is used in fruit and Cherry flavors at the rate of about 0.5 to 10 ppm, calculated on the finished product.

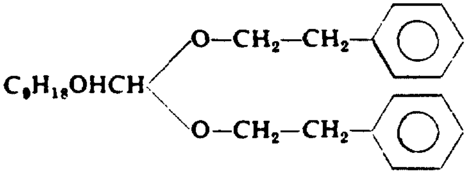
G.R.A.S. F.E.M.A. No.2585.

FCC-1964-837.

Prod.: by condensation of Hydroxycitronellal with Methanol, using dry Hydrochloric gas a condensing agent.

4-64; 33-158; 86-62; 106-191; 156-182; 156-190;

## 1732: HYDROXYCITRONELLAL DIPHENYLETHYLACETAL



$C_{26}H_{38}O_3 = 398.59$

Colorless viscous liquid. Sp.Gr. 0.93. B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Very mild floral odor, producing a rosy effect in compositions, but barely showing an odor of its own. Excellent tenacity.

This Acetal, an almost obvious member on the research chemists' program, does not really offer any unique or outstanding odor or effects in a perfume composition. It is used in Muguet bases, where it is of paramount importance that the floral theme is a delicate, subdued and very tenacious one. It also helps in the green-floral portion of the Muguet theme.

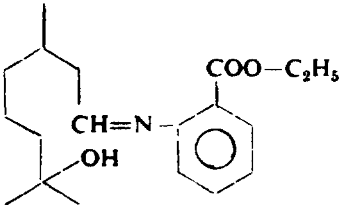
Apart from such isolated fields of application, there is not much need for this Acetal.

Prod.: by condensation of Hydroxycitronellal and Phenylethyl alcohol.

4-64;

## 1733: HYDROXYCITRONELLAL-ETHYLANTHRANILATE

A "Schiff's base".
Ethyl-*N*-*3*,*7*-dimethyl-*7*-hydroxyoctyliden-anthranilate.



$C_{19}H_{29}NO_3 = 319.45$

Intensely yellow, viscous liquid. Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

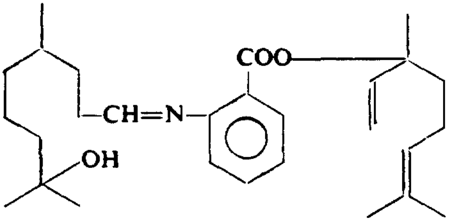
Very sweet, heavy-floral and extremely tenacious odor of Honey-Orangeblossom-Magnolia type.

This base, although closely related to the widely used Methylhomologue, is only rarely used in perfumes or flavors. It forms an excellent base for a Frangipanni (fantasy) fragrance, Magnolia and – naturally – as a modifier in Orangeblossom, Honeysuckle, etc.

It is not often offered commercially under its proper name, but the base is commonly prepared by the individual perfume houses who find it interesting.

Prod.: by condensation of Ethyl anthranilate and Hydroxycitronellal.

## 1734: HYDROXYCITRONELLAL-LINALYLANTHRANILATE



$C_{27}H_{41}NO_3 = 427.63$

Yellow viscous liquid.

Insoluble in water, soluble in alcohol, miscible with oils.

Sweet, floral odor of great tenacity. The odor type varies considerably according to origin (manufacturer and method) of the material.

It is furthermore complicated by the fact that Linalyl anthranilate from manufacturers using "old" process is very far from pure Linalyl anthranilate, and may contain 25% or more of foreign esters and alcohols. It is therefore difficult go give a generally applicable odor description.

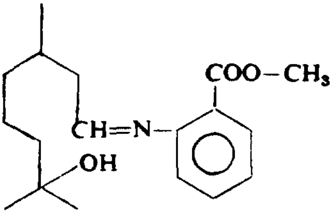
For reasons stated above, this base has – according to the author's impression – largely been abandoned by most perfume houses, and may only exist as an old research sample in a closed cabinet.

It is mentioned as a typical example of the results of "theoretical" thinking in perfumery research. Presumably in the hope that the Lily notes from Linalool-Linalylanthranilate can be combined with the floral Lily notes from Hydroxycitronellal into an fabulous new base, these Schiff's bases are not all so interesting, or rather, they are not always what one would expect them to be.

If the Linalylanthranilate has been prepared via the Dehydrolinalylanthranilate (followed by hydrogenation), there is a good possibility that a true Hydroxycitronellal-Linalylanthranilate can be made. Otherwise, the product will be a very ill-defined one.

## 1735: HYDROXYCITRONELLAL-METHYLANTHRANILATE

A Schiff's base.
Methyl-*N*-3,7-dimethyl-7-hydroxyoctylidene anthranilate.
This material is marketed under a wealth of trade names, of which the most common are listed below:
Aurantiol – Auriol – Auranol – Auralva – Anthralal – Aurangeol – Aurantine – Bigariol – etc., etc.



$C_{18}H_{27}NO_3 = 305.43$

Intensely yellow, viscous to very viscous (see below, Prod.:) liquid, often non-pourable at room temperature.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Very sweet, heavy-floral Orange-blossom to Lindenflower type odor of considerable tenacity. The odor varies with the exact composition of the product (see Prod.: below).

This Schiff's base is the most widely used of all Schiff's bases known in perfumery. Its low cost and considerable strength, its tenacity and versatility are virtues that make the product applicable in fragrances of all price levels and for numerous purposes.

Obviously and almost inevitably used in Orangeblossom, Neroli and related heavy florals, it finds use in smaller amounts in countless other fragrance types: Citrus blends, Ambres, Orientals, Chypres, etc. It forms the steady undertone in many such sweet florals, in Honeysuckle, Frangipanni, Magnolia, exotic florals, etc. In the Citrus Cologne types it has the ability to appear even in the initial notes, besides being a fixative.

Used for nearly 50 years, it has been brought "back to life" several times, e. g. when the fruity-musky perfume was fashionable (and still is, to a certain degree), that perfume had a solid undertone of this type material, backed up by Ethylene brassylate and Undecanolide in unusually high proportions.

This base has perceptible effect in a perfume oil at concentrations beginning well below 1 %, but is often used at much higher level.

Prod.: It is common practice to use a surplus of Methylanthranilate in the condensation process, e. g. from 1.1 Mol. to 1.3 Mol. Anthranilate for each 1.0 Mol. Hydroxycitronellal. In other words, from approximately equal parts by weight to a 130/100 ratio of Methylanthranilate to Hydroxycitronellal.

The theoretical ratio would be 114 parts of Hydroxycitronellal per 100 parts of Methyl anthranilate by weight. When condensation is made in this ratio, the product becomes so viscous, that it is non-pourable at room temperature.

The condensation is carried out under various conditions, e. g. by simple heating to about 90° C. for several hours under stirring, or by more gentle heating under mild vacuum (50-60 mm Hg. pressure) in order to quantitatively remove the water. The theoretical water loss is about 6% of the weight of the reaction mixture.

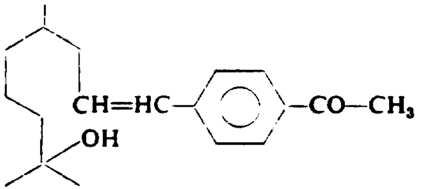
The variations in the ratio of the two components cause considerable variations in the appearance (color and viscosity) and in the odor (from Lily to Orangeblossom). This may be one reason why many creative perfume houses prefer to prepare their own Schiff's bases.

4-19; 17-50; 106-64;

## 1736: HYDROXYCITRONELLIDENE-para-TOLYL METHYL KETONE

*para*-Methylacetophenone-Hydroxycitronellal.

(Theoretical structure):



$C_{19}H_{28}O_2 = 288.43$

Pale yellowish viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Heavy-sweet, herbaceous-floral odor of excellent tenacity. As usual in the case of condensation products, odor differences occur parallel with the proportional use of the components involved in the condensation. In this particular case, variations are quite significant, since only one component supplies the floral notes, while the other tend to appear rather harsh, far from delicate.

The author believes that the original intention with subject material was to produce a Mimosa-type odor in one material. The Acetophenone derivatives are conventionally mentioned in connection with Mimosa, although the chief characteristic of Mimosa is its delicate, light, and utmost discrete odor – far from the agressive harshness of the Acetophenones.

The combination with Hydroxycitronellal is a step in the direction of "taming" the initial harsh notes of the Acetophenones, and in this respect one can say the the subject condensation material serves a purpose and deserves a space on the perfumer's shelf.

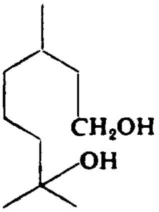
This material blends excellently with the Ionones, with Sandalwood and Cedarwood, and it gives interesting effects with Cinnamic alcohol or Anisalcohol and their derivatives.

This chemical is rarely offered under its proper chemical name.

Prod.: by condensation of Hydroxycitronellal with *para*-Methylacetophenone.

## 1737: HYDROXYCITRONELLOL

*3*,*7*-Dimethyloctan-*1*,*7*-diol.
"Allofixine".
Citronellolhydrate (old name).
Hydroxy dihydrocitronellol.



$C_{10}H_{22}O_2 = 174.29$

Colorless, very viscous liquid. Sp.Gr. 0.93. B.P. 263° C.

Slightly soluble in water, soluble in alcohol and oils.

Very mild (weak) clean-sweet, floral odor of considerable tenacity. The floral type is Rose-Peony, typically less green, less Lily or Muguet than the aldehyde.

Sweet floral taste in dilutions below 10 ppm.

This alcohol, now often manufactured as an intermediate in the production of Hydroxycitronellal, is used in perfume compositions originally with the intention of stabilizing Hydroxycitronellal and prolonging the odor life of that aldehyde in compositions.

However, there are other uses for this alcohol, not always obvious from a brief glimpse at the odor, which is, truly, not immediately impressive. It has an excellent fixative effect upon many types of delicate floral fragrance, and as a blender/modifier for other types.

The use of Hydroxycitronellol as a stabilizer for Hydroxycitronellal is still practised, but the author finds that the alcohol has much wider possibilities and virtues of its own as an odorant.

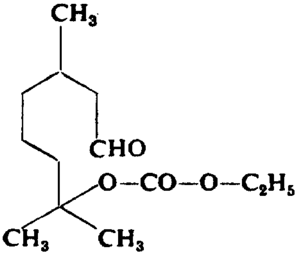
The alcohol is used sparingly in flavor compositions, mainly for imitation Lemon, Lime, Cherry and in various floral flavor themes. The concentration in the finished product may be about 0.3 up to 4 ppm.

G.R.A.S. F.E.M.A. No.2586.

Prod.: (many methods, e. g.): from Myrcene via its Dihydrochloride to Chlorodihydrogeranyl acetate, followed by saponification and hydrogenation to subject alcohol. The method may be used in the manufacture of Hydroxycitronellal (see that monograph).

4-65; 31-25; 86-62; 106-192; 156-182; 156-189;

## 1738: HYDROXYCITRONELLYL ETHYLCARBONATE



$C_{13}H_{24}O_4 = 244.34$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Soft, sweet, balsamic-floral odor with pleasant ethereal overtones and moderate tenacity.

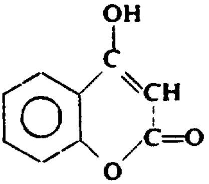
This ester is used in perfume compositions, but rarely offered commercially under its proper chemical name. It offers sweet and mildly floral undertones of a type that blends well with musky odors, e. g. for powder perfumes, etc.

A large number of Ethylcarbonates have been produced and many of them have become quite popular as "foundation" notes in modern fragrances. Their versatility and, in many cases, good tenacity, makes them nearly ideal for base material in new creations.

Prod.: from Hydroxycitronellol plus Ethyl alcohol plus Ethyl chloro formate.

## 1739: 4-HYDROXY COUMARIN

An isomer of Umbelliferone.



$C_9H_6O_3 = 162.15$

Colorless or white crystals. M.P. 212° C.

Practically insoluble in water, soluble in alcohol and oils.

Very faint woody-medicinal odor with a nut-like, herbaceous tone.

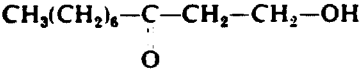
This material has been suggested for use in perfumery, but the author is of the impression that it could hardly find any other application than that of a fixative. It produces little or no odor of its own even when evaluated in compositions. At higher concentrations (it is not very soluble in alcohol and oils) it tends to introduce a dry, almost medicinal odor which can hardly be classified as desirable in a fragrance.

Prod.:

1) from Methylacetylsalicylate by internal condensation using Sodium in liquid paraffin at 240° C.
2) from *ortho*-Hydroxy acetophenone plus Ethylcarbonate plus Sodium.
3) from Diphenyl malonate by cyclization with Aluminum chloride.

69-878; 163-347;
see also *4*-Methoxy coumarin.

## 1740: 1-HYDROXY-3-DECANONE



$$CH_3(CH_2)_6-\underset{\underset{\displaystyle O}{\|}}{C}-CH_2-CH_2-OH$$

$C_{10}H_{20}O_2 = 172.27$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, somewhat fungoid or mushroomy odor, in dilution reminiscent of Amylvinylcarbinol and related Lavender trace materials.

The subject ketol is rarely offered as such commercially, but it may occur as part of various reaction mixtures intended for use in soap perfumery as Lavender-reinforcing agents.

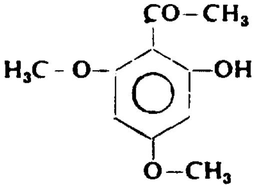
It is most conceivable that these ketols will appear from time to time in perfume compositions, but it is also likely that newer versions will be produced, and other become obsolete.

Prod.: in general, these materials are produced as *beta*- or *1,3*-ketols by the condensation of formaldehyde with various ketones, first of all the ketones already known to have Lavender effects: Methyl hexyl ketone, Ethyl amyl ketone, Methyl heptyl ketone, etc. The condensation leads to primary *1,3*-ketols, and the perfume material may or may not be a single, well-defined chemical.

See also: *3*-Hydroxymethyl-*2*-nonanone.

## 1741: 2-HYDROXY-4,6-DIMETHOXY ACETOPHENONE

Phloracetophenone dimethylether.
Xanthoxylin.
Brevifolin.



$C_{10}H_{12}O_4 = 196.21$

Colorless or white crystals. M.P. 84° C.
B.P. 307° C.

Insoluble in water, soluble in alcohol and oils.

Dry-woody, camphoraceous-medicinal type of odor. Very good tenacity.

This Phenolether has been suggested for use in perfume compositions perhaps more because it has been identified in several natural products, rather than because of its actual perfumery value.

Beyond being a fixative and "another dry-woody" material, it has not much to offer the perfumer, and the author has his doubts about the future of this item. Most likely it will become obsolete in perfumery. It could find limited application in artificial Oakmoss or Oakmoss bases, but even in that field there are better materials available.

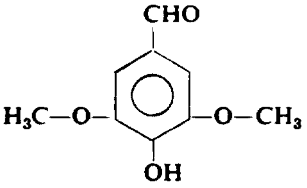
Prod.: by regulated (Di)methylation of Phloracetophenone with Dimethylsulfate in weak aqueous alkali.

36-1255; 68-755; 103-275; 90-541;
See also monograph No. 981.

## 1742: 4-HYDROXY-3,5-DIMETHOXYBENZALDEHYDE

Syringic aldehyde.
*5*-Methoxyvanillin.
Gallusaldehyde-*3,5*-dimethylether.
*3,5*-Dimethoxy-*4*-hydroxybenzaldehyde.
"Dimethylgallic aldehyde".

NOTE: Do not confuse with: *para*-Tolyl acetaldehyde (*para*-Methyl phenylacetaldehyde) which is commercially called Syringa aldehyde.



$C_9H_{10}O_4 = 182.18$

Colorless or white crystals. M.P. 113° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, balsamic-floral odor of considerable tenacity. It has notes in common with Vanillin but is not as sweet and not as Vanilla-like, more floral and slightly greener.

Although this material is very closely related to many widely used perfume and flavor materials, it has not achieved much popularity and is rarely offered commercially by the usual manufacturers of perfume and flavor chemicals.

One reason for its poor success may be the cost of production which is inevitably higher than that of Vanillin.

Prod.:

1) from Pyrogallol-*1,3*-dimethylether by Reimer-Tiemann reaction.
2) from Dimethoxy phenylallylether via Claisen rearrangement to *6*-Methoxy-*iso*-eugenol, followed by isomerization and oxidation to subject material.

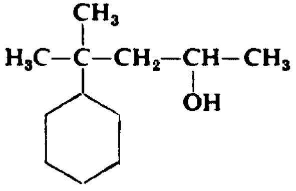
The corresponding alcohol, Sinapyl alcohol, is one of the major breakdown products of naturally occurring Lignin. It can be oxidized to subject aldehyde.

See also monograph on: Coniferyl alcohol (No. 703).

68-750; 37-92;

## 1743: 2-HYDROXY-4,4-DIMETHYL-4-CYCLOHEXYL BUTANE

*alpha-alpha*-Dimethyl hexahydrophenylethyl methylcarbinol.
*alpha-alpha*-Dimethyl cyclohexylethyl methylcarbinol.
*4*-Methyl-*4*-cyclohexylpentan-*2*-ol.



$C_{12}H_{24}O = 184.32$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful dry-camphoraceous odor with a slightly floral undertone and moderate tenacity.

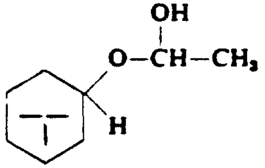
This material has been suggested for use in perfume compositions particularly in soap perfumes, where its stability and relative economy should be of interest. It has also been used as an extender for Vetiver oil in soap perfumes.

It is rarely offered commercially, and only occasionally under its proper chemical name.

Prod.: by hydrogenation of *2*-Hydroxy-*4,4*-dimethyl-*4*-phenylbutane.

See also: (4-109); 163-202;

## 1744: 2-HYDROXYETHYL-2-BORNANYLETHER



$C_{12}H_{22}O_2$ = 198.31

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-camphoraceous-minty, Lime-like odor of moderate to poor tenacity.

This material, only recently developed, finds some use in the reconstruction of essential oils (artificial essential oils), particularly in Lime oil (distilled Lime type).

With the enormous increase in demand for distilled (and, to a lesser degree, expressed) Lime oil, any material, useful in the duplication of the Lime odor should be welcome. However, the title material has not at this time (August 1968) been commercially marketed.

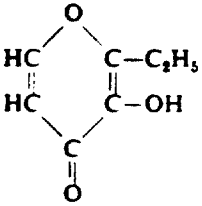
For use in artificial Lime oil intended for flavors, the material would need the approval of the respective authorities before it could be incorporated in food flavors.

Prod.: from *beta*-Pinene via Camphene.

(The Glidden Co. Div. of S.C.M. Corp. 1967).

## 1745: 3-HYDROXY-2-ETHYL-4-PYRONE

"Ethyl Veltol" (Pfizer).
"Veltol Plus" (Pfizer).
"Ethyl Palatone" (misleading name).
*3*-Ethyl-*2*-hydroxy-*4H*-pyran-*4*-one.



$C_7H_8O_3$ = 140.14

White crystalline powder. M.P. 89 to 93° C.

Soluble 1.6% in water at room temperature, better in warm water, 12% soluble in alcohol, 5% in Phenylethylalcohol, 5½% in Propylene glycol.

Intensely sweet, fruity-breadlike, pleasant odor of immense tenacity in spite of considerable volatility at room temperature.

Sweet, fruity-jamlike taste, reminiscent of Pineapple, Strawberry, Vanilla and heavy fruit-preserve or syrup, depending upon the concentration.

Although its flavor is somewhat similar to that of Palatone (the lower – Methyl – homologue), the subject material is more breadlike, less caramellic, softer, sweeter and much longer lasting. Its taste is sweeter, less distinctly Pineapple-Strawberry-like, more fruit-and-bread like, and overall more delicate, uniform.

The manufacturer claims that this material is 4 to 6 times stronger than its lower homologue. The author agrees that with respect to sweetness in flavor compositions, it compares to 3 to 5 times the amount of Palatone, while in perfumes it seems to be about 4 times stronger or rather, it is 4 times more tenacious and has a similar, but more delicate and uniform odor performance. One of its greatest assets is that of being an enhancer of sweetness, indirectly reducing the need for sugar in the flavored product. This effect is obviously of considerable interest to the beverage manufacturers in our days of "diet-soda" drinking.

The better solubility in alcohol is also an advantage over Palatone, and the water solubility of interest to the flavor industry.

Hydroxy ethylpyrone is used in perfume compositions as a sweetener at very low concentrations, while at slightly higher levels it may support fruity notes or floral-fruity notes (in Jasmin, Tuberose, etc.). Its enormous tenacity may cause surprises to the unexperienced perfumer trying this material, but adequate fixation of a base including the subject material should ensure proper performance and no "sticking out" in the terminal notes.

An entirely novel application is the use at 5 to 15 ppm in Tomato catsup and Tomato soup. The effect here is that of a flavor enhancer and a co-sweetener. Other applications are, e. g. 5 to 50 ppm in Chocolate toppings and desserts and 1.5 to 6 ppm in various beverages.

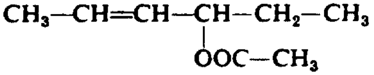
G.R.A.S. (Approved for food use in the U.S.A. 1968).

Prod.: See also: Maltol.

Pfizer data sheet No. 635, April 1967.

## 1746: 4-HYDROXY-2-HEXENYLACETATE

A confusing*) commercial name for:
*secondary*-Hexenyl acetate
Ethyl butenylacetate.
An isomer of "Leaf alcohol" acetate.



$$\mathrm{CH_3{-}CH{=}CH{-}\underset{\substack{|\\ OOC-CH_3}}{CH}{-}CH_2{-}CH_3}$$

$C_8H_{14}O_2 = 142.20$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

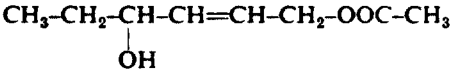
Powerful ethereal, fruity-green, vinous odor of poor tenacity.

This ester was once suggested for use in perfume compositions, but the industry has seen so many - and better - materials for similar odor purposes during the past two decades, that the title ester, and many other unusual chemicals related to it, have become almost obsolete.

The subject material seems to be unavailable at the time of writing this monograph. It is mentioned for the sake of completion on the subject of "green" Hexenyl-derivatives.

Prod.: from *4*-Ethyl-*2*-buten-*4*-ol with Acetic acid.

*) Confusing, because the title name would call for the structure:



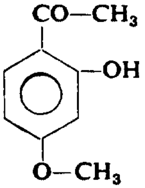
$$\mathrm{CH_3{-}CH_2{-}\underset{\substack{|\\ OH}}{CH}{-}CH{=}CH{-}CH_2{-}OOC{-}CH_3}$$

$C_8H_{14}O_3 = 158.20$

but the author feels that commercial samples have referred to the structure given under the title name.

## 1747: 2-HYDROXY-4-METHOXYACETOPHENONE

*4*-Acetylresorcinol monomethylether.
"Peony Ketone".
Paeonol.
Peonol.
Resacetophenone-*4*-methylether.
"Paeonal".
*para*-Methoxy-*ortho*-hydroxy phenylmethyl ketone.



$C_9H_{10}O_3 = 166.18$

Colorless or white needles. M.P. 50° C. B.P. 256° C. Volatile with steam.

Almost insoluble in water, soluble in alcohol and oils.

Warm-aromatic odor, rather pungent and not typically reminiscent of any specific natural material. Somewhat haylike, also remotely floral, heavy and sweet, with good tenacity.

This ketone is not often offered commercially, and not often found on the perfumer's shelf. Although it is milder than the conventional derivatives of Acetophenone, it has still some harshness, typical of that chemical family, and it lacks naturalness. Its name may lead the observer to believe that it possesses a Peony odor, but unfortunately it does not. The chemical is present in a number of essential oils and extracts, mainly from the underground parts of certain plants, otherwise not used in perfume or flavor.

It could find use in New Mown Hay compositions, in certain types of heavy florals and in various soap perfumes, where its relative power may be helpful. It carries one phenol-group and is subject to the same hazards of discoloration, etc. as most other phenols.

Prod.:

1) from Resorcinol monomethylether plus Acetonitrile with Zinc chloride and Hydrochloric acid.
2) by partial Methylation of Resacetophenone.

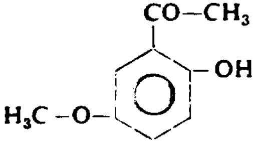
36-1255; 68-754; 90-538; 103-275;
see also: Acetovanillone (28).

NOTE: several literature sources list "2-Hydroxy-4-methoxy *acetone*". The author believes that this is a typographical error, and reference is actually made to the *Acetophenone*-derivative.

See also: 981 and 1741.

## 1748: 2-HYDROXY-5-METHOXY ACETOPHENONE

*ortho*-Acetylhydroquinone monomethylether.
Quinacetophenone-5-methylether.



$C_9H_{10}O_3 = 166.18$

Yellowish prismatic crystals. M.P. 50° C.

Almost insoluble in water, soluble in alcohol and oils.

Aromatic, somewhat medicinal, warm, woody-herbaceous odor of good tenacity. It is not as sweet as the *2,4*-isomer (see previous monograph), and just as far from any known natural odor.

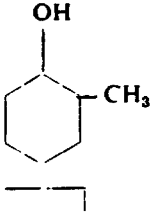
This material could find some use in perfume compositions, e. g. in artificial Oakmoss, in New Mown Hay fragrances, and in certain heavy florals. It blends well with Labdanum and with the Lavender type oils, and it lends a certain amount of power and undertones to the fragrance. It is not frequently offered commercially from the usual producers of fragrance chemicals, but is often available from manufacturers of Acetophenone derivatives and Alkoxybenzene chemicals.

Prod.: by controlled Methylation of Quinacetophenone with Dimethylsulfate in weak aqueous alkaline solution.

90-539; see also: Acetovanillone (No. 28).

## 1749: 1-HYDROXY-2-METHYL-4-tertiary-AMYLCYCLOHEXANE

*ortho*-Methyl-*para-tertiary*-amylcyclohexanol.



$C_{12}H_{24}O = 184.32$

Colorless, viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Woody-rootlike, dry-sweet and very tenacious odor with resemblance to Vetiver, Cedar and Amyris.

This material has been suggested for use in perfume compositions, where it may introduce a supporting note to Vetiver and precious wood notes, furthermore give "lift" and stable power – particularly in soap perfumes. It blends excellently with the Ionones and Methylionones, with Cedarwood derivatives and musks, and with Oakmoss products.

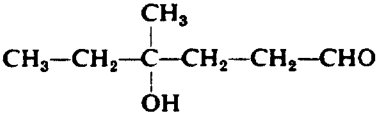
It is rarely offered under its proper chemical name, and many specialties consisting almost entirely of this chemical, may have sophisticating trace additives included to divert the perfumer's attention in certain directions when he first smells the material.

Prod.: by hydrogenation of *ortho*-Methyl-*para-tertiary*-amylphenol.

Note: The acetate of subject secondary alcohol has been produced, but is, to the author's knowledge, not commercially marketed.

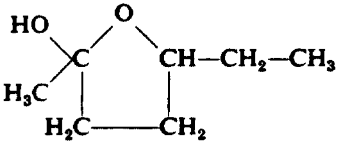
## 1750: gamma-**HYDROXY**-gamma-**METHYL**-n-**CAPROIC ALDEHYDE**

*3*-Hydroxy-*3*-methylhexanal.
Butyraldol.



$$CH_3{-}CH_2{-}\overset{\displaystyle CH_3}{\underset{\displaystyle OH}{C}}{-}CH_2{-}CH_2{-}CHO$$

exists mainly in the cyclic form:



$C_7H_{14}O_2 = 130.19$

Colorless oily liquid.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Fresh-green, oily and slightly floral odor, particularly in dilution. Moderate tenacity, and the odor shows considerable variations from one sample to another, presumably on account of rather poor stability.

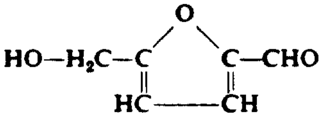
This aldehyde has been suggested for use as part of various fresh topnotes in perfume compositions, mainly in Citrus-type topnotes and foliage bases. It should be properly blended with other green or Citrus-type materials before being incorporated in a perfume. It may have a tendency to "grow" on top of the perfume and override the topnotes, eventually ruining them.

The subject material is believed to be a major component of various successful topnote specialties, but it is rarely offered under its proper chemical name. With recent development of series of "green" materials, it has lost much of its original interest.

Prod.: by condensation of Propionaldehyde and Butyraldehyde.

## 1751: 5-(**HYDROXYMETHYL**)-2-**FURALDEHYDE**

*5*-(Hydroxymethyl)-*2*-furfural.
*5*-(Hydroxymethyl)-*2*-furancarbonal.
*5*-(Hydroxymethyl)-*2*-formylfuran.
"H.M.F.".
Sometimes called Hydroxymethylfur*furol*.



$C_6H_6O_3 = 126.11$

White crystal needles. M.P. 33° C.
Sp.Gr. 1.21 (liquid). B.P. 246° C.

Soluble in water, alcohol, Propylene glycol and in most oils.

Warm-herbaceous, winey-ethereal odor, remotely resembling that of Hungarian Chamomile (Matricaria-oil). Samples from different suppliers show considerable odor difference. A natural sweetness is common, a similarity to Hay and Caramel, Tobacco etc. is often perceptible.

The taste is sweet, herbaceous-Hay-like, mildly tobacco-like. The power is, in the author's opinion, not nearly as impressing as described in many literature sources and publications. In fact, it is quite disappointing, if one *reads* these odor descriptions *before* smelling and tasting the material.

Its water-solubility may be partly responsible for its weak odor, but it could still have a powerful taste.

This material has been suggested for use in flavor compositions to enhance the flavor of Honey, Tobacco, Bread, etc.

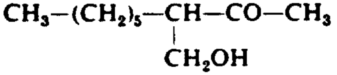
Although it has not been identified as such in a natural, unprocessed food product, it appears to be present in Honey, Tobacco and freshly baked bread, etc.

Prod.: from Fructose, obtained from sugar.

NOTE: This material will, unless highly diluted, cause a yellow coloring of human skin when applied. The effect resembles that of Dihydroxyacetone and many other hydroxy-ketones or hydroxy-aldehydes, particularly those with ethylenic linkage and/or ring structure.

90-776; 100-541; 158-162;

## 1752: 3-HYDROXYMETHYL-2-NONANONE



$$CH_3{-}(CH_2)_5{-}\underset{\substack{|\\ CH_2OH}}{CH}{-}CO{-}CH_3$$

$C_{10}H_{20}O_2 = 172.27$

Colorless oily liquid.

Warm-herbaceous, slightly musty-mushroom-like odor with nut-like undertones and moderate tenacity.

This material is probably not marketed as such, but it forms part of various specialties, usually appearing as mixtures of several isomers as produced by the reaction in which they are formed.

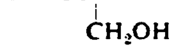
The isomer-mixture is used in soap perfumes as modifiers and supporting notes for herbaceous fragrances, particularly Lavender.

– See also: *1*-Hydroxy-*3*-decanone.

Prod.: (various methods, e. g.) by hydrogenation of a condensation product from Heptaldehyde and Acetone.

## 1753: 3-HYDROXYMETHYL-2-OCTANONE

See also: *1*-Hydroxy-*3*-nonanone (1756).



$$CH_3(CH_2)_4\underset{\substack{|\\ CH_2OH}}{CH}{-}CO{-}CH_3$$

$C_9H_{18}O_2 = 158.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Musty-herbaceous, sweet, slightly earthy odor of moderate tenacity.

The subject material occurs mainly as part of a reaction mixture and is rarely offered as an individual fragrance chemical.

The mixture finds some use in soap perfumes as a blender and fortifier for Lavender and other herbaceous fragrance types.

Prod.: by condensation of Methyl hexyl ketone with Formaldehyde, followed by hydrogenation.

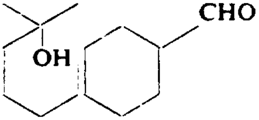
See also the related materials: *1*-Hydroxy-*3*-decanone, and: *3*-Hydroxymethyl-*2*-nonanone.

# 1754: 4-(4-HYDROXY-4-METHYL PENTYL)-3-CYCLOHEXENE-10-CARBOXALDEHYDE

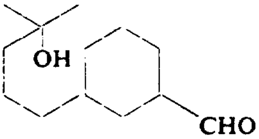
*4*-(*4*-Methyl-*4*-hydroxyamyl)-*3*-cyclohexene carboxaldehyde.

"Lyral" (I.F.F.).

The commercial product under the name "Lyral" (I.F.F.) is a mixture of two isomers:



and



$C_{13}H_{22}O_2 = 210.32$

Colorless viscous liquid, barely pourable at room temperature. Practically insoluble in water, soluble in alcohol and oils.

The viscosity increases further upon exposure to air, daylight and excessive heat, probably causing polymerization and decomposition.

The odor is delicately sweet, light and floral with outstanding tenacity and a radiation which surprises most first-time observers. There are people who will claim that they can not smell this material, but upon a closer study it will usually become evident, that this aldehyde has power and volume underneath the delicate olfactory surface.

"Lyral" only recently celebrated its 10th anniversary, and it may already rank among the "upper ten" of the truly new aromatic chemicals of our generation as far as volume is concerned. This in itself is an achievement which speaks clearly for the success of the aldehyde. It has not been identified in Nature, and most conceivably never will be, judging from the structure and the chemical family to which it belongs.

Lyral was at first believed to be of fixative value only, e. g. in high-class soap perfumes, etc. But it was soon discovered that Lyral has a floral volume which, when properly "cultivated" by the creative perfumer, often outperforms Hydrocitronellal and any other floral chemical or combination of chemicals.

Its application is therefore continously expanding from the single floral Muguet to become the "must" in cosmetic fragrances where tenacity and sweet-powdery, stable terminal notes are called for. It blends excellently with the Ionones and with the conventional resinoids (Styrax, Tolu, Peru, etc.) and it may either accompany Hydroxycitronellal or substitute it. It is generally agreed that it is distinctly superior to Hydroxycitronellal in overall effect and stability.

Lyral is higher boiling than Hydroxycitronellal and seems to be more stable under normally mild, alkaline conditions. It forms "Schiff's bases" with Anthranilates, and condensation products with Indole, Skatole, Quinolines and a few other perfume materials.

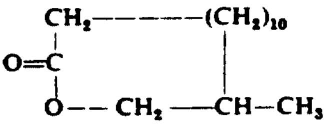
The normal use concentration will be from 1 or 2% as a floral modifier or part-fixative to 6, 8 or 10% in typically floral and tenacious fragrances. The present market price of Lyral is about twice the price of Hydroxy-citronellal.

Prod.: Myrcene is the starting material in the patented process. This terpene is condensed with Acrolein under heat to yield *4*-(*4*-Methyl-*3*-penten-*1*-yl)-*3*-cyclohexene-*1*-carboxaldehyde (see that monograph) followed by hydrogenation and hydroxylation to subject aldehyde.

Alternatively, Myrcene may be reacted into Myrcenol which in turn is condensed with Acrolein in a Diels-Alder type condensation. Hydrogenation yields Lyral.

156-370;

## 1755: 14-HYDROXY-13-METHYL-1-TETRADECANOIC ACID, LACTONE



$C_{15}H_{28}O_2 = 240.39$

Colorless viscous oil. B.P. 270° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Rich, sweet, musky odor of good tenacity. Not quite as delicately "animal" as Cyclopentadecanolide, and not nearly as retentive on the skin "in-use", but of an overall good and typical musky odor in the perfumery sense.

The title material is mentioned as an example of many isomers and homologues, some of which are listed below:

*14*-HYDROXY-*1*-METHYLTETRADECAN-*1*-OIC ACID, LACTONE:
*14*-HYDROXY-*2*-METHYLTETRADECAN-*1*-OIC ACID, LACTONE
*14*-HYDROXY-*14*-METHYLTETRADECAN-*1*-OIC ACID, LACTONE

all of which have Musk odors of type and power sufficient to qualify them as perfume chemicals.

Prod.: from the Glycolester or Glycerol ester of the respective acid. Lactonization may be undertaken by heating with Sodium methoxide.

31-187; see also: 156-264;

## 1756: 1-HYDROXY-3-NONANONE

$CH_3$—$(CH_2)_5$—CO—$CH_2$—$CH_2$—OH

$C_9H_{18}O_2 = 158.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, somewhat earthy or Walnut-like, sweet odor of moderate tenacity.

This ketone is not offered as an individual chemical, but appears as a major part of a mixture of ketones in a commercial product.

The product is intended for use in herbaceous fragrance types, particularly those intended for soap. It enhances the odor fo Lavender and blends excellently with Labdanum, Opopanax, Geranium, Coumarin and with most of the spice oils, etc.

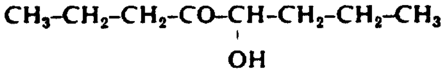
The slightly fatty-oily notes of the material (mixture) itself, is generally not perceptible once the mixture is incorporated in a fragrance. The oily notes can be utilized with advantage in Lavender-Lavandin compositions, and in Bergamot bases.

Prod.: by condensation of Methyl hexylketone and Formaldehyde, followed by hydrogenation.

(See also: *3*-Hydroxymethyl-*2*-octanone).

## 1757: 5-HYDROXY-4-OCTANONE

Butyroin.
*5*-Octanol-*4*-one.



$CH_3\text{–}CH_2\text{–}CH_2\text{–}CO\text{–}\underset{\displaystyle OH}{CH}\text{–}CH_2\text{–}CH_2\text{–}CH_3$

$C_8H_{16}O_2 = 144.22$

Pale yellowish or almost colorless liquid.
B.P. 182° C. Sp.Gr. 0.91.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and slightly pungent-buttery-nut-like odor.

Sweet buttery taste with a pleasant oily mildness at concentrations below 5 ppm. The flavor is not as sharp as that of Dibutyryl or that of Acetyl caproyl ($C_8H_{15}O_2$).

There is little, if any, use of this material in perfume compositions.

It finds some use in flavor compositions, particularly in imitation Butter, Butterscotch, Cheese, Buttermilk, Nut, Fruit, etc.

The concentration used is normally about 0.5 up to 10 ppm. High concentration of sugar, Vanillin or other sweeteners may often allow for much higher concentrations of Butyroin.

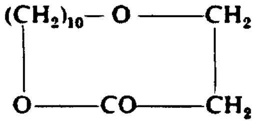
G.R.A.S. F.E.M.A. No.2587.

Prod.: from Ethylbutyrate in Ether solution by reaction with Sodium.

26-448; 66-710; 100-184; B-I-840;

## 1758: 14-HYDROXY-4-OXY-TETRADECYLLACTONE

*4*-Oxa-tetradecanolide.



$C_{13}H_{24}O_3 = 228.29$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol, miscible with oils.

Strong and tenacious musky odor. The Musk note is deficient in delicate animal tones, inferior in performance on the human skin, and does not seem to enhance a fragrance picture, the way Cyclopentadecanolide can do it.

A very large number of macrocyclic musks have been developed in search of inexpensive versions of the desirable "Exaltolide"-effect, but very few truly successful musks have come out of this tedious and expensive research program.

The title Lactone is mentioned as one example of a lower homologue of a series, in which certain higher members have become quite successful and are gaining strong foothold on many perfumers' shelves.

(See Oxahexadecanolide).

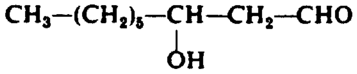
Apart from possible "captive" use by certain manufacturers, there is probably very little of the named Oxalactone used in today's perfumery.

Prod.: from Chloro-undecanol plus Acrylonitrile.

50-204; 156-264;

## 1759: beta-HYDROXY PELARGONIC ALDEHYDE

*beta*-Hydroxynonanal.
Caproaldol.
Hexyl hydracrylic aldehyde.



$$CH_3-(CH_2)_5-\underset{\displaystyle OH}{\underset{|}{CH}}-CH_2-CHO$$

$C_9H_{18}O_2 = 158.24$

Colorless or very pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Oily-pungent, somewhat cheesy-nut-like odor, overall rather unpleasant. The herbaceous notes are concealed in an oily character which leans toward the rancid note.

This aldehyde has been suggested for use in flavor compositions, e. g. Cheese, Nut, Butter, etc. but does not seem to have attained any success in this field.

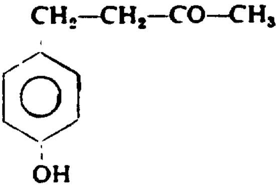
It is, to the author's knowledge, not used in perfumery.

Prod.: by Aldol-condensation of Acetaldehyde and Heptaldehyde.

4-110;

## 1760: para-HYDROXY PHENYLBUTANONE

*4-(para-*Hydroxyphenyl)-*2*-butanone.
"Oxyphenylon" (I.F.F.).
"Oxanone" (Dragoco).
"Frambinone, cryst."
"Raspberry ketone".
"Rasketone".
*para*-Hydroxybenzyl acetone.
*para*-Hydroxyphenylethyl methyl ketone.



$C_{10}H_{12}O_2 = 164.21$

White needle-like crystals or granular crystalline material.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet, fruity and warm odor resembling Raspberry preserve and having a moderate tenacity.

Sweet-fruity taste but not very powerful (contrary to what is often said about this chemical). Concentrations below 10 ppm are hardly characteristic and not easy to identify the material by.

Although known for more than 50 years, this chemical was not brought into common commercial use in perfumes and flavors until about 10 years ago. Prior to that, it was an important component of certain well-known flavor (and fragrance) specialties.

This ketone is used in perfume compositions, particularly in Jasmin, Gardenia, Tuberose, etc. where floral notes need fruity undertones, or where fruity notes need fixation and supporting delicate sweetness. One known Jasmin specialty carries a considerable proportion of this material in its "fruit-preserve-like" undertones and terminal notes.

The most important use of Hydroxyphenylbutanone is, however, in flavor compositions, particularly after the indentification of the ketone in Raspberry juice. As a fruity fixative, it finds extensive use in other fruit flavors, e. g. "Tutti-grutti", Strawberry, Pineapple, Peach and in a number of combination flavors.

The concentration used is about 5 to 50 ppm in the finished product and may reach 300 to 350 in chewing gum.

G.R.A.S. F.E.M.A. No.2588.

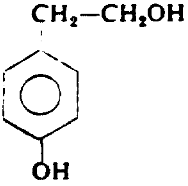
Prod.:

1) from: *para*-Hydroxybenzaldehyde plus Acetone by condensation, followed by hydrogenation.
2) from Phenol plus Methyl vinyl ketone in presence of a catalyst.

156-380; 159-666; 140-167; 159-306;

## 1761: para-HYDROXY PHENYLETHYLALCOHOL

*beta-para*-Hydroxyphenyl ethanol.
Tyrosol.



$C_8H_{10}O_2 = 138.17$

White crystalline powder. M.P. 93° C.
B.P. 294° C.

Slightly soluble in water, soluble in alcohol and most oils.

Faint, sweet fruity-floral odor, mainly rosy.

Sweet, but very weak taste, rather nondescript.

This material has only recently entered the flavor laboratories, and perhaps more because of its presence in natural Raspberry juice than on account of its individual odor and flavor.

The Methylether of subject material is also used in flavor compositions, but it is not commercially offered under its proper chemical name.

The two materials are both very weak as

flavors, and play a minor role in Raspberry and a few other fruit flavors, partly a fixative role.

Prod.:

1) from Tyrosine by biological synthesis.

2) from *beta-para*-Hydroxy phenylethylamine plus Nitrous acid.

68-736;

## 1762: beta-HYDROXYPROPIONIC ALDEHYDE-iso-AMYLETHER

Hydracrylic aldehyde-*iso*-amylether.
*beta-iso*-Pentoxypropionic aldehyde.

$(CH_3)_2—CH—CH_2—CH_2—O—CH_2—CH_2—CHO$

$C_8H_{16}O_2 = 144.22$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar warm-herbaceous, almost caramellic odor, yet with little resemblance to a natural product.

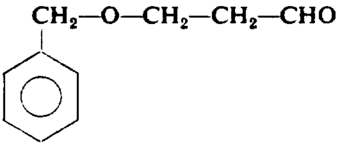
This Oxyaldehyde is a member of a comprehensive series of Etheracetals and Oxyaldehydes, etc., experimentally developed in the 1930's. A few of these have come to regular use. The author has preferred to include some of the materials which do not seem to have achieved acceptance by the perfume industry in order to complete the general picture of the series.

Prod.: from *beta*-Hydroxypropionic aldehyde plus *iso*-Amylalcohol.

(Berichte 1935, vol. 68, page 838).

## 1763: beta-HYDROXYPROPIONIC ALDEHYDE BENZYLETHER

Hydracrylic aldehyde benzylether.
*beta*-Benzoxy propionic aldehyde.



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Musty-herbaceous, rather sweet odor of moderate tenacity.

Subject Oxyaldehyde is, in the author's opinion, one of the least interesting of the series. See comments under previous monograph.

Prod.: from *beta*-Hydroxypropionic aldehyde plus Benzylalcohol.

## 1764: beta-HYDROXYPROPIONIC ALDEHYDE DIETHYLACETAL-iso-AMYLETHER

*beta-iso*-Pentoxypropionaldehyde diethylacetal.

$(C_2H_5O)_2CH—CH_2—CH_2—O—CH_2—CH_2—CH(CH_3)_2$

$C_{12}H_{26}O_3 = 218.34$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Comparatively powerful, warm-herbaceous-ethereal odor with a peculiar resemblance to Pyridine or Quinoline, yet not nearly as penetrating. Fair to good tenacity.

This Ether-acetal has been suggested for use in perfume compositions as a new note and a modifier in various types of "Men's Fragrances", e. g. Fougères, Moss-bases, "Tabac" fragrances, Leather notes etc.

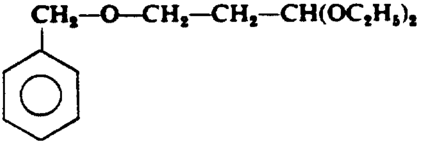
It is rarely offered under its proper chemical name, and it is not commonly used in perfumes.

Prod.: from *iso*-Amylalcohol plus *beta*-Hydroxypropionaldehydediethylacetal.

31-75;

## **1765:** beta-**HYDROXYPROPIONIC ALDEHYDE DIETHYLACETAL BENZYLETHER**

*beta*-Benzoxypropionic aldehyde diethylacetal.



$C_{14}H_{22}O_3 = 238.33$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral, almost rosy and slightly musty-woody odor of moderate to good tenacity.

Suggested for use in perfume compositions as a modifier in Rose fragrances, also for soap perfumes. It gives more sweetness than the Phenyl and Tolyl ethers and less of the "metallic-green" note of those materials.

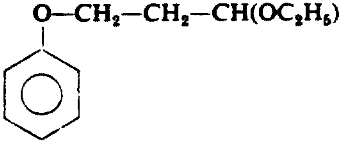
This Ether-acetal is not commonly used in perfumery, but is often encountered in perfumery research and experimental perfumery. It is rarely offered commercially.

Prod.: from Benzylalcohol plus *beta*-Hydroxypropionic aldehyde diethylacetal.

31-75;

## **1766:** beta-**HYDROXYPROPIONIC ALDEHYDE DIETHYLACETAL PHENYLETHER**

*beta*-Phenoxypropionic aldehyde diethylacetal.



$C_{13}H_{20}O_3 = 224.30$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, vegetable-green odor with a floral undertone and good tenacity. Some observers find the odor similar to that of Watermelon.

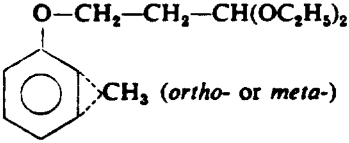
Suggested for use in perfume compositions, mainly in support of "green" topnotes and partly as a fixative in such notes. It performs well with aldehydic-Citrus type fragrances, and also in modern versions of the Fougere theme, where freshness is desirable rather than the conventional, overly sweet and extremely tenacious Salicylate theme. This Ether-acetal gives interesting effects with Geranium and with Cyclamen aldehyde, Hydroxycitronellal and Methoxycitronellal, etc.

It is rarely offered under its proper chemical name.

Prod.: from Phenol plus *beta*-Hydroxypropionic aldehyde diethylacetal.

31-75;

## **1767:** beta-**HYDROXYPROPIONIC ALDEHYDE DIETHYLACETAL**-meta-(and ortho-)-**TOLYLETHER**



$C_{14}H_{22}O_3 = 238.33$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

The *ortho-* and the *meta*-isomers have sweet, floral-balsamic odors while the *para*-isomer is so weak that it can be classified as absolutely uninteresting, except for academic studies.

A product containing a mixture primarily of the *ortho-* and the *meta*-isomer has been recommended for use in soap perfumes.

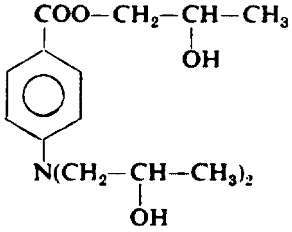
This product has considerable stability except in strongly acid media.

Subject material is rarely offered under its proper chemical name.

Prod.: from Cresol (isomer mixture) plus *beta*-Hydroxypropionicaldehydediethylacetal.

31-75;

## 1768: 2-HYDROXYPROPYL-para-N,N-bis (2-HYDROXYPROPYL) AMINOBENZOATE



$C_{16}H_{25}NO_5 = 311.38$

The title chemical has been discussed in literature and listed as a fragrance chemical, but the author of this work has only included the material because it finds use as a preservative with mild antioxidant effect (indirectly) upon perfume solutions to prevent deterioration of the perfume oil and the alcohol.

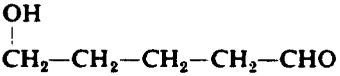
It is deplorable to observe the number of perfumes, colognes and other alcoholic perfume oil solutions currently in the market, with very clearly perceptible notes of oxidation, rancidity or other sign of deterioration which could easily be inhibited or almost prevented.

Apparently, it has not yet become customary to "follow" the finished product on its way to the customer. Many perfumes and colognes contain ingredients which have oxidizing effect upon the alcohol or upon other ingredients in the fragrance. Ionones are particularly active, and so is Citral, etc. An alcoholic solution of Ionone will smell of Acetaldehyde after amazingly short time of ordinary storage. Needless to add that such volatile trace ingredient is capable of completely "overriding" a fine perfume and destroy the immediate impression of its fragrance.

With the excellent and very efficient antioxidants available today, and a choice of combination-antioxidants for every purpose, there is really no excuse for sending functional products unprotected on the market.

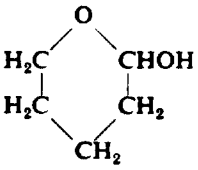
## 1769: delta-HYDROXY VALERIC ALDEHYDE

This aldehyde exists largely in the cyclic form:



$\overset{\text{OH}}{\text{CH}_2}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CHO}$

or:



$C_5H_{10}O_2 = 102.14$

Colorless liquid.

Slightly soluble in water, soluble in alcohol and oils.

Very mild, herbaceous-haylike odor with variable amounts of rootlike or pungent notes. The author believes that samples submitted for evaluation have been of questionable purity.

According to the physical conditions in a composition, this aldehyde may act as an alcohol or as an aldehyde. Such flexibility is not exactly appreciated by the perfumer or flavorist, although the phenomenon is by no means uncommon.

The title material has been suggested for use in the reconstruction of certain essential oils, and as a trace component in perfume compositions of hay- or tobaccolike character.

The material is not listed in the U.S. Federal Register or mentioned in the G.R.A.S list of F.E.M.A. Accordingly, it should not be used for food flavors in the U.S.A.

Prod.: by hydrogenation of 5-Hydroxyvaleric acid.

(See also: 66-706; 66-801).

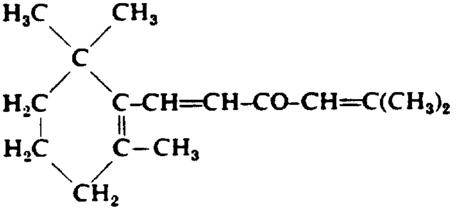
## 1770: IANTHONE

Janthon.

A trade name for an Ionone-type chemical: *6*-(*2,6,6*-Trimethyl-*1*-(or-*2*-) cyclohexen-*1*-yl)-*1*-methyl-*2,5*-hexadien-*4*-one.

*iso*-Propylidene ionone.

NOTE: This structure describes the *beta*-isomer



$C_{16}H_{24}O$ = 232.37

Almost colorless or pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Powdery-dustry, dry, Orris-like odor of considerable tenacity.

This ketone, one of many higher homologues of Ionone, has been suggested for use in perfume compositions, and has been commercially available for several decades.

The fact that it is not widely used may indicate that it does not quite live up to its original promises, but it may also indicate that newer derivatives have given the perfumer more exactly or to a higher degree what he was looking for, at a more reasonable cost.

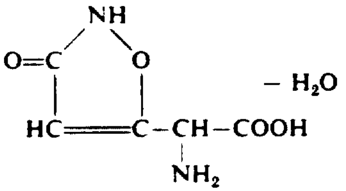
Yet, there are not too many materials of the kind that enables the perfumer to create the highly desirable "powdery" notes in fine perfumes, and it is worthwhile holding on to the few we have.

This ketone includes a good fixative effect, and performs beautifully in Cassie compositions and in Ambre type fragrances.

Prod.: by condensation of Citral with Mesityloxide (*iso*-Propylidene Acetone) followed by cyclization. The resulting product contains at least two isomers, one of which is pictured in above structure.

4-74; 7-215; 89-388; 156-203;
See also No. 1377 = *beta*-Euionone, an isomer.

## 1771: IBOTENIC ACID



$C_5H_6N_2O_4$ = 158.12
(anhydrous)

White powder or solid, white mass.

Soluble in water and alcohol. Poorly soluble in oils.

Practically odorless. Faint, meat-like, mild and sweet taste in aqueous dilutions.

This material is used in flavor compositions or, rather, in the food additives industry as a synergist to the comparatively new flavor-enhancers: Sodium guanylate and Sodium inosinate.

The individual effect of subject acid is approximately 20 ppm and higher, meaning that this is near minimum effective strength of the material if no other flavor enhancer is added.

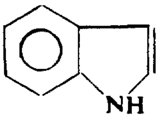
It is quite conceivable that this material will play an increasing role in modern flavor additives, following the Glutamates and the guanylate – inosinates.

Prod.: isolated from the Japanese fly mushroom. The acid can be produced synthetically.

158-270;

## 1772: INDOLE

*2,3*-Benzpyrrole.
Benzopyrrole.
*1*-Benzazole.



$C_8H_7N = 117.15$

White crystal flakes. M.P. 52° C.
B.P. 254° C. (decompos.).

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils. Slightly soluble in hot water.

Extremely diffusive and powerful odor, almost tarry-repulsive and choking when concentrated, but in concentrations lower than 0.1 % or in compositions, it shows powerful floral notes and pleasant radiation. Good tenacity, in spite of the volatility at room temperature.

Concentrations below 0.2 ppm have fairly pleasant taste, but the effect is strongly dependant upon the presence of other flavor materials, and their flavor character.

Indole is widely used as a floralizer in Jasmin, Lilac, Neroli, Gardenia and numerous other heavy or exotic flower bases and fragrance types. Concentrations may reach several percent in Jasmin bases, while in Muguet the delicate components cannot allow such high concentration of Indole, usually 0.1 to 0.4 %. Traces of Indole may be used to give a "lift" without adding the pungency which accompanies higher amounts of this material.

By its chemical Nature, Indole may cause some problems in perfumery when incorporated with aldehydes, etc. In some cases, a condensation process leads to a new product, a change in color and viscosity, in other cases the odor and color change is so perceptible that it may be undesirable.

The sensitivity of Indole to daylight is well known to the perfumer, and the problems of incorporating Indole in a perfume intended for a white soap has been discussed for decades. Manufacturers of Indole and some perfumers seem to agree, that at least a great part of the problem is due to trace impurities in the Indole, not to Indole itself. It is also beyond doubt that today's soap cake is far superior to the soap made 10 or 20 years ago, and the wrapping in multiple paper and foil layers was a great step towards safer soap perfuming – and an open door to the use of many materials previously avoided in soaps.

The ability of Indole to discolor aldehydes or to become discolored in their presence is sometimes quite impressive. And since Indole is often shipped in plastic-lined cardboard containers (Indole discolors in presence of Iron), it may permeate the container and its vapors may travel far to cause damage to other materials. Aldehydes and ketones, paticularly the crystalline ones, may discolor even when stored at a considerable distance from Indole. Heliotropine and Hydroxyphenylbutanone are typical examples of such sensitive aldehydes and ketones.

But with proper packing, and thinkful handling, many of these problems can be overcome. The perfumer will know not to add solid Indole to Heliotropine in the dry state in the beginning of a formula make-up. It is wise to keep the Indole aside and add it when the composition is complete or nearly complete, i. e. at the time of highest dilution of the troublesome components. It is in such cases that a chemistry background comes in handy to the perfumer, since many of his "aldehydes" do not even carry a name or a syllabus that indicate that they are aldehydes.

In the perfume laboratory, it is common practice to have Indole only in the shape of a 10% or 5% solution in Diethyl phthalate or other innocuous solvent. The mere presence of Indole crystals even in the most meticulously closed and cleaned glass jar, is a hazard to the odor purity of the perfume laboratory. And the spilling of a few crystal leaflets of Indole may disturb the odor of a perfume laboratory for days or weeks unless they are quantitatively removed.

Indole is used in flavor compositions, in concentrations much lower than those in perfumes. It finds its way into imitation Chocolate, Raspberry, Strawberry, Bitter Orange, Coffee, Nut, Cheese, Violet, Grapefruit, etc. and in fruit complexes.

The concentration is equivalent to about 0.02 to 0.50 ppm in the finished product. The problem of discoloration of Indole in flavors is neglegible, since the concentration is so low that dilution alone protects against hazardous chemical contact.

G.R.A.S. F.E.M.A. No.2593.

Prod.:

1) from Indigo in the process of making that coloring material.
2) by isolation from coal tar.
3) from Benzol plus *ortho*-formotoluide in Potassium hydroxide solution, followed by cyclization.
4) from Ethyl-*ortho*-formate plus *ortho*-Toluidine followed by treatment of the Formamidine with Potassium Butoxide.

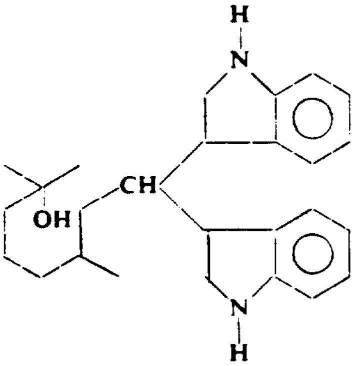
4-65; 69-81; 85-70; 86-63; 106-193; 156-192; 100-554; 26-586; 95-202; 96-221; B-XX-304; 90-812;

## 1773: INDOLENE

The name "Indolene" is used by a number of perfume chemical manufacturers and it has been applied to many specialties. This monograph describes the chief or active ingredient in the commercial product called Indolene, originally from Roure-Bertrand Frères et Justin Dupont, later marketed by many other companies.

"Indolique" (Fritzsche Bros., Inc.).

*8,8*$^{bis}$-(*3H*-Indol-*3*-yl)-*2,6*-dimethyl-*2*-octanol.



$C_{26}H_{32}N_2O = 388.56$

Straw-colored or pale amber-colored, rarely pale straw-colored, extremely viscous liquid, not pourable at room temperature. Commercial products are often diluted with Diethylphthalate or other inert solvent to make the product pourable and handy and to protect the Indolene from harmful intermittent heating.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

The odor varies considerably according to the manufacturer's method of processing, ratio of components, etc. and also the age of the product plays an important role.

Freshly prepared Indolene with a near-perfect chemical balance has a mild, delicate, but extremely tenacious floral odor of considerable radiation. The Indole-type topnote can be adjusted to suit the perfumer, but the original purpose of the product was to avoid Indole as such, or to create a "battery" charged with Indole for controlled release of that powerful floral odor over a very extended period.

The use of Hydroxycitronellal in surplus may seem to solve the problem of having "free" Indole-notes, but it does not beautify the product. Most perfumers seem to prefer a perceptible Indole note over a rich, sweet-floral background.

There exists some differences of opion as to the exact chemical Nature of Indolene. In any event, the commercial name does not apply to a well-defined chemical, and Indolene from different sources of manufacture can rarely be used interchangeably.

Indolene is widely used in perfume compositions, not only in floral bases, Muguet, Jasmin, Tuberose, Hyacinth, Narcisse, etc. but also as an enriching floralizer with great fixative effect. It may assist in the fixation of Oriental or Chypre bases, as it can be used in relatively high percentage. Although Indolene is chemically equivalent to about 60% Indole, one can often use 2 to 5 parts of Indolene for each one part of Indole originally intended – and with a similar floralizing effect plus an increased floral fixative effect. Which should prove that Indolene is an individual chemical, not a physical mixture.

Certain perfume specialties contain Indolene as a major part of a complex, also containing Phenylacetaldehyde-derivatives, etc. and certain Glycol acetals.

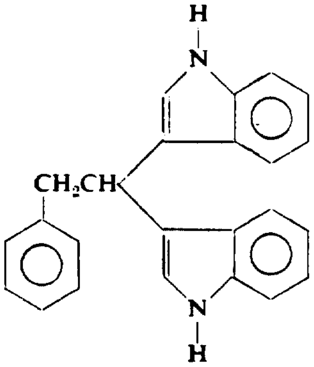
Prod.: Indolene is manufactured from (theoretically) 2 Mol. Indole plus 1 Mol. Hydroxycitronellal by condensation under heating.

The proportions may vary slightly, and it is common practice to add Diethyl phthalate to the mixture prior to heating, so that the condensation product is somewhat protected against local overheating, and the finished product becomes light of color and fairly pourable at room temperature.

## 1774: INDOLE-PHENYLACETALDEHYDE

*beta-beta-bis-(3H*-Indol-*3*-yl)-*alpha*-phenylethylene.

"Di-indolyl phenylethylene".



$C_{24}H_{20}N_2 = 336.44$

Viscous, pale straw-colored or pale amber-colored liquid. Viscosity and color may increase to non-pourable and brown appearance with age or improper storage conditions.

Insoluble in water, soluble in alcohol and oils.

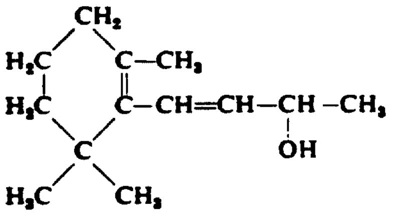
Powerful, sweet-floral and very tenacious odor of Hyacinth-Honeysuckle character. The odor varies considerably according to the ratio of the two components used, and the method of production. It is common practice to include about 50% Diethylphthalate in the product to make it handy, pourable and more stable.

This product is used in perfume compositions where an effect of Phenylacetalderyde along with that of Indole is desirable and high fixation wanted. The floral notes and the heavy, sweet-earthy notes of the two components are combined in a single body of unusual richness and with the effect subdued and prolonged. It is possible to use considerably higher percentages of this material than one could expect from stoechiometric calculations on the Indole content. Which proves that the Indole is indeed chemically combined into a new material.

Although far from being as popular as the Indolene, this material has found some use in heavy florals, Fougères, Chypres, Hyacinth bases, Honeysuckle and Lilac, etc. It seems to discolor more readily than Indole.

Prod.: From Indole and Phenylacetaldehyde, theoretically in the ratio of 2 Mol. Indole to 1 Mol. Phenylacetaldehyde. It is customary to include Diethylphthalate in the amount equivalent to 50% of the finished product.

## 1775: beta-IONOL



$C_{13}H_{22}O$ = 194.32

Almost colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, oily-herbaceous, warm odor with floral-balsamic undertones. There is some resemblance to Labdanum notes and the tenacity is moderate.

This secondary alcohol has been suggested for use in perfume compositions as a modifier in various types of floral and non-floral fragrances. It blends well with Labdanum, Lavender, Lavandin, Clary Sage, etc. and it has a refreshing effect upon Rose types. It performs pleasantly with the alifatic aldehydes into refreshing notes varying from Pine to Rose, and it was at one time used in several types of detergent fragrances. However, it seems to have lost its importance, and it is still too expensive to become a large-volume material in household fragrances etc.

Prod.: by reduction of *beta*-Ionone with Sodium alcoholate or by Meerwein-Ponndorf-Verley reduction.

30-277; 89-386;
(Hoffmann-laRoche, 1959).

## 1776: IONONES, summary

The following Ionone-type materials are included in this work under the numbers indicated; referring to individual monographs:

| | |
|---|---|
| 86 | Allyl ionone. |
| 95 | Allyl pulegone. |
| 698 | Citrylidene allylacetone. |
| 699 | Citrylidene cyclopentanone. |
| 765 | Dimethyl ionone. |
| 766 | *alpha*-Methyl ethyl ionone. |
| 769 | Cyclogeranyl methylketone. |
| 947 | *cis*-Dihydro ionone. |
| 948 | Dihydro-*alpha*-ionone. |
| 949 | Dihydro-*beta*-ionone. |
| 950 | Dihydro-*gamma*-ionone. |
| 951 | Dihydro-*alpha*-irone and Dihydro-*iso-alpha*-irone. |
| 952 | Dihydro-*beta*-irone. |
| 953 | Dihydro-*gamma*-irone. |
| 961 | Dihydro-*alpha*-methyl ionone. |
| 962 | Dihydro-*delta*-methyl ionone. |
| 1001 | *1*-(*2,3*-Dimethyl cyclohexyl)-*1*-buten-*3*-one. |
| 1002 | *1*-(*3,5*-Dimethyl cyclohexyl)-*1*-buten-*3*-one. |
| 1274 | *alpha*-Ethyl ionone. |
| 1357 | *alpha*-Ethyl-*2,2,6*-trimethyl cyclohexane butyric aldehyde. |
| 1377 | *beta*-Euionone. |
| 1588 | Hexahydro pseudoionone. |
| 1770 | Ianthone. |
| 1777 | *alpha*-Ionone. |
| 1778 | *beta*-Ionone. |
| 1779 | *gamma*-Ionone. |
| 1780 | *beta*-Ionone epoxide. |
| 1781 | *alpha*-Ionone ethylglycidate. |
| 1782 | *alpha*-Ionone methylanthranilate. |
| 1783 | *alpha*-Ionone methylglycidate. |
| 1784 | *alpha*-Irone. |
| 1785 | *beta*-Irone. |
| 1786 | *gamma*-Irone. |
| 1973 | *4*-(*1*-Methyl-*3*-cyclohexenyl)-*3*-buten-*2*-one. |
| 1975 | *1*-(*6*-Methyl-*3*-cyclohexenyl)-*1*-penten-*3*-one. |
| 2084 | *alpha*-Methyl ional. |
| 2085 | *alpha-n*-Methyl ionone. |
| 2086 | *alpha-iso*-Methyl ionone. |
| 2087 | *beta-n*-Methyl ionone. |
| 2088 | *beta-iso*-Methyl ionone. |
| 2089 | *gamma-n*-Methyl ionone. |
| 2090 | *gamma-iso*-Methyl ionone. |
| 2091 | *4*-Methyl ionone. |
| 2092 | *5*-Methyl ionone. |
| 2109 | *5*-Methyl-*1*-(*3*-methyl-*3*-cyclohexenyl)-*1,3*-hexanedione. |
| 2250 | Methyl trimethyl cyclohexenyl butenal. |

2251 *3*-Methyl-*4*-(*2*,*4*,*6*-Trimethyl-*3*-cyclohexenyl)-*3*-buten-*2*-one.
2312 Neo-irones (four isomers).
2456 Pentione.
2762 Pseudo ionone.
2764 Pseudo methyl ethyl ionone.
2765 Pseudo methyl ionone.
2766 Pseudo-*iso*-methyl ionone.
2907 Tetrahydro ionone.
2925 Tetrahydro pseudo ionone.
2996 *4*-(*2*,*6*,*6*-Trimethyl-*6*-cycloheptenyl)-*3*-buten-*2*-one.
3002 *4*-(*2*,*4*,*6*-Trimethyl-*3*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.
3004 *1*,*1*,*8*-Trimethyl-*2*-cyclo octanone.
3011 *2*,*6*,*6*-Trimethyl-*1*,*2*,*3*,*4*-tetrahydro benzalacetone.

Not included in this work are:
*alpha*-Acetyl Ionone (from Acetylacetone plus Citral).
*alpha*-Propenylionone.
*alpha*-*iso*-Amylenionone.
*alpha*-*iso*-Ionone (Terpinolenyl acetone).

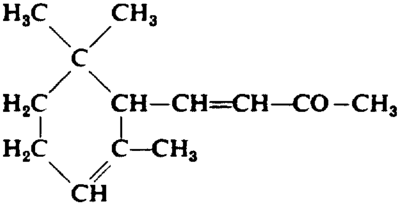
## 1777: alpha-IONONE

*4*-(*2*,*2*,*6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.

Note: The name "Ionone", also including the "Methylionone" was used by the original producers of these ketones, Haarmann & Reimer in Germany. Ketones, identical to these, but manufactured by other companies, were named with different trade names, and the name "Ionone" was protected by registration by the original producers. However, the name was not protected in all countries, and the use of the name "Ionone" has become international in description of these ketones, regardless who is the manufacturer. The Haarmann & Reimer patents covering the manufacture of Ionones are now more than 75 years old, and the world production of these ketones is far in excess of five million pounds per year.

The author has preferred to use the name "Ionone" in description of these ketones in the belief that this name is the best known and most commonly used. Trade names have been left out for the reason that there are simply too many types, grades and qualities, all carrying different names and all being basically a type of an Ionone or a mixture of isomer Ionones.

Ionones are listed in this work under the letter "I", while Methylionones are listed under the letter "M". A few, better known and more widely used homologues or related Ionones and related Alkyl-ionones are listed under their chemical name or the most common trade name, all cross-indexed in the index in volume No. 2.



$C_{13}H_{20}O = 192.30$

Almost colorless or pale straw-colored to pale yellowish oily liquid. Sp.Gr. 0.93. B.P. 237° C.

Very slightly soluble in water, soluble in alcohol and oils, slightly soluble in Propylene glycol. With to-day's improved distillation equipment, a "white" or virtually colorless product is possible. Commercial grades are rarely colorless.

Warm-woody, balsamic-floral odor of deep sweetness and moderate tenacity. Its resemblance to the odor of Violet flowers is legendary.

Relatively powerful, sweet-woody taste with a fruity note. Higher concentrations – e. g. 20 ppm and up – tend to be "perfumey", slightly bitter and overly woody-floral.

*alpha*-Ionone is used widely in perfume compositions of almost all types. It is many decades since the single floral Violet note was appreciated as a fragrance for cosmetic purposes, but Ionone has found numerous other applications. The use of Ionone in Rose bases is very common and generally well liked, and smaller amounts of Ionone are used in woody, herbaceous, floral, balsamic, piney or Citrus-like fragrances. It is almost not possible to name a fragrance in which Ionone has not been tried for modifications, blending, floralizing, mellowing, etc. It is often part of the highly desirable complex that displays "powdery" undertones in a fragrance.

*alpha*-Ionone, like most other Ionones, has a noticeable effect of temporarily fatiguing the human sense of olfaction. Perfumers know this, and learn to smell Ionones with caution, not inhaling their fragrance deeply or repeatedly.

Ionones are not extremely stable. Upon prolonged storage they develop sour or harsh topnotes, their color and viscosity increase, and their solubility in alcohol is impaired. Many Ionones contain antioxidants or other breakdown-retarding additives, but it is generally considered wise to re-check the odor quality of Ionones and Methylionones every 3 to 6 months according to storage conditions.

*alpha*-Ionone is also used in flavor compositions, mainly in imitation Berry compositions, Blackberry, Loganberry, Raspberry, Cherry, etc. and in Spice blends, fruit complexes (for chewing gum, etc.) Citrus flavors, floral flavors and Vanilla imitation.

The concentration used is about 2 to 50 *ppm* in the finished product. One peculiar application of Ionone is that of accompanying Anethole, Menthol and Licorice extract in certain types of Licorice candy. A related use is the very old type of "Sen-Sen" flavor for the tiny Licorice pellets used as "Mouth-fresheners" since the turn of the century.

Prod.:

1) from Citral by condensation with Acetone, followed by cyclization.
2) from *De*hydrolinalool plus Ethyl acetoacetate by Carroll's synthesis to Pseudo Ionone, followed by cyclization.

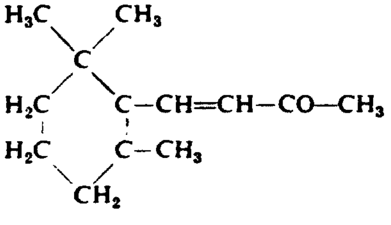
There are countless variations of these methods with very intricate details aimed at increasing the yield of one or the other isomer.

G.R.A.S. F.E.M.A. No.2954.

4-77; 31-92; 34-806; 36-1037; 36-1145; 51-73; 67-502; 77-211; 26-588; 86-79; 89-368; 95-166; 96-166; 103-268; 156-198; B-VII-168;

## 1778: beta-IONONE

*4*-(*2,6,6*-Trimethyl-*1*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.



$C_{13}H_{20}O = 192.30$

Almost colorless or very pale straw-colored oily liquid. Sp.Gr. 0.95. B.P. 239° C.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

NOTE: see comprehensive notes on "Ionone" under *alpha*-Ionone, previous monograph.

Warm, woody, somewhat dry odor with a fruity undertone. There is some degree of disagreement between perfumers as to the "fruity" note. Not all perfumers find it fruity, and the general preference for one Ionone over the other as a perfume material also seems to vary. The common viewpoint is that *beta*-Ionone resembles Cedarwood and has a Raspberry-like undertone, while *alpha*-Ionone is the more typical Violet odor, sweeter, and less green than the *beta*-isomer.

*beta*-Ionone is used in perfumery although not to the same extent as *alpha*-Ionone. The high production figures published in annual statistics for *beta*-Ionone include the amounts used in the Vitamin A industry, amounts which may exceed the net volume used in perfumes and flavors. It finds its way more into fragrances rich in woody notes, including those employing newer derivatives of Cyclohexanol, etc. It is also more widely used in lipstick fragrances on account of its compatibility with fruity fragrance materials, particularly Raspberry chemicals.

*beta*-Ionone is also used in flavor compositions for imitation Berry (Raspberry, Loganberry, Strawberry, Cherry), Grape, Muscatel, Nut and fruit complexes, Pistacio, Pineapple, in floral complexes and Liqueur flavors. It is used in its highest concentrations in Licorice candy and in chewing gum. Normal concentrations are 1 to 10 ppm in the finished product, and up to 100 ppm in chewing gum.

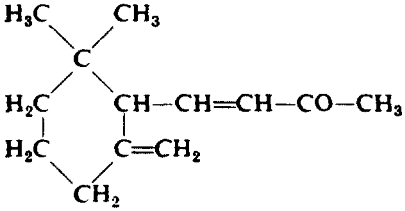
The taste is less sweet, more "perfumey" and more fruity than that of *alpha*-Ionone, quite powerful, and not pleasant beyond 10 ppm unless other flavor materials are present.

G.R.A.S. F.E.M.A. No.2595.

26-588; 31-92; 36-1037; 36-1145; 85-73; 89-368; 95-166; 96-166; 103-268; 106-194; 156-198; B-VII-167;

## 1779: gamma-IONONE

*4*-(*2*-Methylene-*6*,*6*-dimethylcyclohexyl)-*3*-buten-*2*-one.



$C_{13}H_{20}O = 192.30$

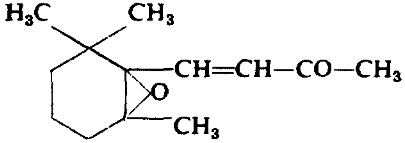
This ketone is mentioned only for the sake of completing the picture of Ionone isomers.

It is – to the author's knowledge – not commercially available but occurs as a trace component in commercial grades of *alpha*- and *beta*-Ionone, and it could be isolated or brought into commercial scale production if the demand for such isomer should occur or increase.

89-368; 156-198;

## 1780: beta-IONONE EPOXIDE

Epoxy-*2,3*-*beta*-ionone.
Sometimes called:
*beta*-Ionone-*5*,*6*-epoxide.



$C_{13}H_{20}O_2 = 208.30$

Pale yellowish or almost whitish crystalline mass or white crystals. M.P. 48° C. B.P. 262° C.

Intensely sweet, fruity-woody odor of great volume and excellent tenacity, suggestive of precious woods with floral background notes and a similarity to Raspberry.

The material acquires an acetic odor if exposed to air and daylight, but it is otherwise extremely stable, and far superior to the Ionones in that respect.

This oxide was identified in the gases above stored, preserved carrots and also in the storage piles of Guinea palm fruits. The two naturals both contain Carotene, a Pro-vitamin A, which is derived from Ionone as an intermediate in the biosynthesis of Vitamin A.

Many years later, the oxide was synthesized and repeatedly offered to the perfume industry, but with very little success. Recent improvements in the synthesis of Ionones have also yielded useful improvements in the preparation of the epoxides, and they are once again offered commercially.

The title material finds some use in compositions, particularly in soaps and detergents, where its greater stability gives it advantage over the conventional Ionones. It blends excellently with Ambregris-chemicals, Musks, Labdanum, Sandalwood materials, Cinnamic alcohol (for "powdery notes"), etc. and it gives very interesting variations in the "Origan" type fragrances, known for their high Ionone content with *iso*-Eugenol, etc.

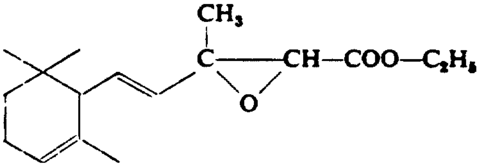
It could find use in flavor compositions, particularly Raspberry and Strawberry imitations, but the material is not yet named as G.R.A.S. in the official American lists.

Prod.: from Epoxy-citral, which is derived from Citral by oxidation with Hydrogen peroxide.

86-50; 158-147; 163-196;

## 1781: alpha-IONONE ETHYLGLYCIDATE

Ethyl-*alpha*-ionone glycidate.
Ethyl-*2,3*-epoxy-*3*-methyl-*5*-(*2,6,6*-trimethyl-*2*-cyclohexenyl)-*4*-pentenoate.



$C_{17}H_{26}O_3$ = 278.40

Yellowish or pale amber-colored viscous liquid.

Insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Very sweet, deep, warm-fruity and tenacious odor with a woody undertone. Strikingly reminiscent of the odor of dried figs, dates or dried bananas. Often described as "jam-like".

Sweet fruit-preserve-like taste in dilutions below 10 ppm.

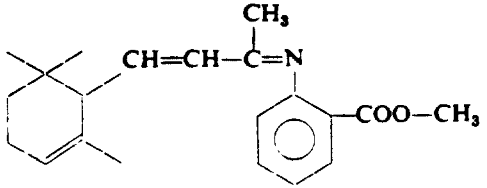
This material, rarely offered under its proper chemical name, and often appearing as a mixture with above chemical as chief component, is occasionally used in perfume compositions. It is particularly suitable for lipstick perfumes and certain types of cream perfume, etc. where lasting, sweet-fruity notes are desirable.

It is also interesting in heavy florals, such as Gardenia, Honeysuckle and Frangipanni.

The subject material finds some use in flavor compositions, particularly in Raspberry imitation for baked goods or hard candy, where the fixative effect of this material comes to use. Although imitation Fig or Date is not frequently called for, it is interesting to observe the odor similarity of this item to the natural materials although most conceivably it is not present in those natural products.

## 1782: alpha-IONONE METHYLANTHRANILATE

An ill-defined, incomplete condensation product.



$C_{21}H_{27}NO_2$ = 325.46

Yellowish viscous oil.

Insoluble in water, soluble in alcohol and oils.

Heavy and very sweet-floral, "Oriental"-balsamic odor of excellent tenacity. Products from different sources of supply show considerable variations in odor characteristics. It is most conceivable that many products under above name contain smaller amounts of "bouquetting" perfume materials. It is also likely that the title material is marketed as chief component of perfume specialties under trade name.

The subject material represents one of many "Schiff's base" type products in which the Anthranilate is combined to a ketone. In the late 1920's and early 1930's, a great number of so-called condensation products were developed from interesting perfumery ketones with Anthranilates. The results were almost never encouraging, since similar results could be achieved by using the two components separately in the respective perfume composition, instead of the "condensation product".

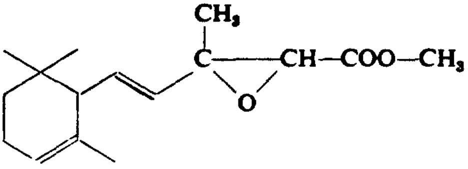
It is most conceivable that this and similar products will become obsolete in perfumery.

Prod.: by "condensation" of equal molecular proportions of *alpha*-Ionone and Methylanthranilate.

The structure above describes the theoretical result from such condensation.

## 1783: alpha-**IONONE METHYLGLYCIDATE**

Methyl-*2,3*-epoxy-*3*-methyl-*5*-(*2,6,6*-trimethyl-*2*-cyclohexenyl)-*4*-pentenoate.
Methyl-*alpha*-ionone glycidate.
Cyclocitralone.



$C_{16}H_{24}O_3 = 264.40$

Pale yellowish to pale amber-colored, viscous liquid.

Insoluble in water, soluble in alcohol and oils. Almost insoluble in Propylene glycol.

Sweet-fruity, caramellic-marmelade-like odor with woody undertones and good tenacity. There is a distinct resemblance to the odor of dried Figs, Dates, Prunes and similar fruit preserve.

The taste is sweet, fruit-preserve-like and rich, with a floral-woody undertone at concentrations below 10 ppm.

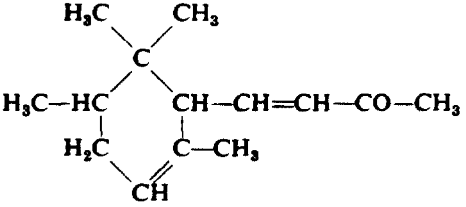
This material is often sold under trade names and has been known for several decades. It is used in certain types of perfume compositions where fruity notes of good tenacity are desirable, and in a few heavy floral fragrance types.

It is also used in flavor compositions, such as Raspberry, Plum, imitation Fig, Date, etc. although in the U.S.A. it is not listed specifically in the G.R.A.S. list.

31-97; 86-79;

## 1784: alpha-**IRONE**

*6*-Methyl-*alpha*-ionone.
*cis*-(*2,6*)-*cis*-($2^1$,$2^2$)-*alpha*-Irone.
*4*-(*2,5,6,6*-Tetramethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.



$C_{14}H_{22}O = 206.33$

Colorless or very pale straw-colored oily liquid. Sp.Gr. 0.94. B.P. 248° C.

Almost insoluble in water, soluble in alcohol and oils.

There are several types and grades of this ketone commercially available and sold under names including the word "*alpha*-Irone". A relatively pure *alpha*-Irone is a very expensive chemical, and there is some tendency among perfumers to accept a product, rich in *alpha*-Irone and with the balance being related Irones that do not greatly disturb the olfactory picture of the desirable *alpha*-isomer.

The odor is soft, warm, Orris-Violet-like, sweet and extremely diffusive. Its true power and effect is clearly demonstrated in dilutions or in active use at concentrations near one percent in a perfume composition. The "lift" and the radiance introduced by this ketone are its greatest assets and advantages to compensate for its high cost.

The taste is sweet, very powerful and, in proper dilution, fruity-berry-like.

With skilful use and blending with the proper Ionone derivatives, it is possible to fully utilize the Irone, but its perfumery application remains restricted by cost and, unfortunately, lack of experience in the use of this exquisite material.

In flavors, where cost of trace components have less influence upon the final cost of the flavor, this material finds quite extensive application. Particularly useful in Raspberry, it is frequently used in other Berry formulations, in fruit complexes, floral (Violet) flavors, etc.

The concentration will normally be equivalent to about 1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2597.

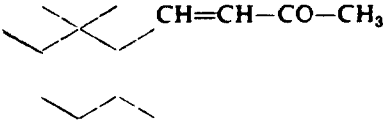
Prod.:

1) by isolation from the volatile oil of Orris rhizomes.
2) from *2,3*-Dimethylhepten-*2*-one-*6*, by addition of Acetylene, followed by partial hydrogenation, via *5*-Methylgeraniol or related chemicals to Pseudo-irone. The use of different mineral acids in the following cyclization monitors the ratio of the yield of various isomers. There are 20 possible isomers, many of which have been prepared on a small, commercial scale from time to time.

4-67; 5-178; 5-336; 31-98; 31-99; 77-212; 86-64/71; 67-504; 26-588; 31-298; 89-395; 100-567; 95-169; 96-165; 106-197; 156-371; 65-466; B-VII-169;

## 1785: beta-**IRONE**

*5*-Methyl-*beta*-ionone.



$C_{14}H_{22}O$ = 206.33

This ketone, rarely offered separately in commercial quantities, is generally regarded as the least interesting of the three best known isomers of Irone.

It is also the isomer that is easiest removed from the mixture of isomers resulting from the synthetic preparation of Irone.

Most perfumers agree that *beta*-Irone resembles *beta*-Ionone in odor except that the Irone is somewhat more powerful.

It is therefore reasonable to conclude that *beta*-Irone has little or no interest to the creative perfumer under the present circumstances and conditions of cost.

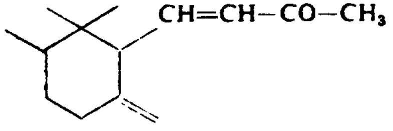
Prod.: *beta*-Irone occurs in Nature so sparingly that isolation from a natural oil is out of consideration.

The method for synthetic preparation, mentioned under *alpha*-Irone will produce *beta*-Irone in larger amounts if sulfuric acid is used in the cyclization of the Pseudo-irone.

65-466; 31-99; 31-98; 89-395; 95-169; 5-178; 5-336; 26-588; 86-64/71; B-VII-169; 4-68;
NOTE: see also monograph: *alpha*-Irone.

## 1786: gamma-**IRONE**

*5*-Methyl-*gamma*-ionone.



$C_{14}H_{22}O$ = 206.33

Colorless or almost colorless oily liquid.
B.P. 251° C. Sp.Gr. 0.94.

Almost insoluble in water, soluble in alcohol and oils.

Warm, soft, woody-Violet-like odor, generally considered slightly weaker and not as radiant as that of *alpha*-Irone.

This isomer, by some workers considered

to be an important ingredient in natural volatile oil of Orris rhizome, has achieved very little interest among the creative perfumers. Its main role will probably be that of contributing notes to a mixture of Irone isomers in order to arrive at the most attractive Violet-like nuances.

In this respect, *gamma*-Irone may be the second-most important next to the *alpha*-Irone.

However, for general use in perfume compositions, it seems at the time of revising this monograph (April 1968) that only *alpha*-Irone can be economically feasible.

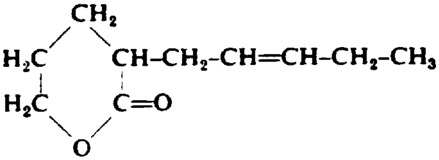
The exact composition of the Irone mixture in natural Orris oil has not yet been clearly or irrevocably elucidated, and one of the chief contributors to our knowledge on Irones has claimed that the presence of *gamma*-Irone in the natural oil is of minor importance, or, rather, dependant upon the geographical origin of the oil.

Prod.: by isolation from the volatile oil of Orris rhizome, preferably from oils in which this isomer occurs abundantly. It has also been prepared synthetically from Pseudoionone.

4-68; 5-178; 5-336; 31-98; 65-466; 86-66; 89-395;
(see also notes under monograph: *alpha*-Irone)

## 1787: JASMINE LACTONE

Sometimes called: Jasmone Lactone.
*cis-5-(2*-Pentenyl-pentanolide-*5,1*).



$C_{10}H_{16}O_2 = 168.24$

Almost colorless oily liquid. B.P. over 300° C. Sp.Gr. 1.01.

Practically insoluble in water, soluble in alcohol and oils.

Powerful oily-fruity, rather fatty and tenacious odor with floral petal-like notes. There is some resemblance to the odor of refined Linseed oil, and the fruity notes resemble Peach or Apricot.

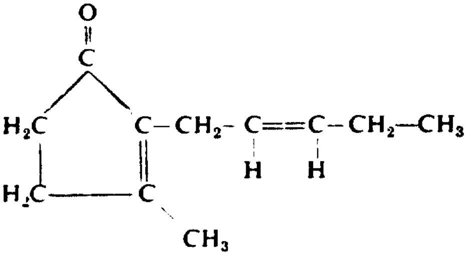
The subject Lactone, identified in Jasmin absolute, has recently become commercially available, but its cost prevents extensive use of the material. However, its main mission so far has been that of filling in one more "missing link" in the olfactory picture of artificial Jasmin absolute.

In the author's opinion it is, however, not always essential to employ exactly the chemicals already identified in Jasmin absolute in order to arrive at the desirable olfactory picture. Sometimes, the "unconventional use" of materials other than those existing in the natural product, can lead to quite remarkable similarity and faithful reproduction of odor. Needless to add that this method of operation may be considerably less expensive, and it might encourage the perfumer in offering a more artistical route to a successful product.

Helvetica Chim. Acta 1962, 1250, page 1256.
(See also: 156-223) 90-355; 105-588;

## 1788: cis-JASMONE

*3*-Methyl-*2*-(*cis*-*2*-penten-*1*-yl)-*2*-cyclopenten-*1*-one.
The naturally occurring Jasmone.



$C_{11}H_{16}O = 164.25$

Pale yellowish or pale straw-colored oily liquid. B.P. 248° C. Sp.Gr. 0.94.

Almost insoluble in water, soluble in alcohol and oils.

Diffusive, warm-spicy, somewhat fruity, but in dilution more floral odor of good tenacity. Its beauty is truly demonstrated in dilutions below one percent, or in modest amounts in a perfume composition. The pure material has notes reminiscent of Celery seed, some find it "bread-like", others find it "fruity", "waxy" etc. Evaluation of a powerful odorant should be undertaken by proper dilution of the material so that nuances can be studied without the inconveniences of odor fatigue.

Recent improvements in the synthetic manufacture of *cis*-Jasmone has increased the possibilities for its use. It is no longer restricted to being a component of fine Jasmin bases and artificial Jasmin absolute, but it may find its way into numerous floral fragrance types and many non-floral ones. Its presence in Peppermint and Spearmint oils encourage the use of *cis*-Jasmone in high-grade Mint flavors.

Traces, often mere fractions of one percent in a perfume oil may introduce just that wanted warmth and deep floral note almost unobtainable with other chemicals.

Its flavor power is even greater. Concentrations of about 1 ppm have perceptible effect in many fruit flavors, while naturally, concentrations in Mint flavors are higher.

Prod.: (many methods) e. g. from *cis-3-*Hexenol via *cis-4-*Heptenoic acid.

5-151; 31-86; 34-579; 34-1210; 34-1211; 67-101; 86-77; 89-363; 100-584; 156-223;

## 1789: »iso-JASMONE«

Commercial products under this name are mixtures of several isomer ketones of which:

1) *n*-Hexyl-cyclopenten-*2*-one: is described under DIHYDRO-*iso*-JASMONE. No. 955.
2) *n*-Hexylidene cyclopentanone: is described under *alpha*-HEXYLIDENE CYCLOPENTANONE. No. 1670.
3) *2-n*-HEXYL-*2*-CYCLOPENTEN-*1*-ONE, so-called Dihydrojasmone. No. 1659.

The literature has been very illogical and inconsistent on the subject of nomenclature, identity and odor description of the commercially available *iso*-Jasmones, etc.

One of the main points of disagreement seems to be the preference of isomer 2) as compared to one or more of the isomers which have an unsaturated ring and a saturated side chain.

Yet, it has also been claimed that the hydrogenated product (which may be identical even when prepared from two different unsaturated isomers) has a superior odor.

The author finds that personal opinions on the odor of these materials will not contribute constructively to the problem, and only general odor descriptions are therefore listed.

"*iso*-Jasmone" is a name given to commercial products of very widely different composition. The fact that there are several "price-levels" also emphasize the difference in opinion as to which odor is closest to that of natural Jasmone, and which is the most desirable for general perfumery use.

Although *iso*-Jasmone is quoted in literature with a chemical structure formula, commercial products are composed of at least two major components, some *iso*-Jasmones have more than four major components.

*iso*-Jasmones are used widely in perfumes and flavors, and the very attractive cost of certain isomer blends has contributed to an extensive use of these ketones in quite ordinary perfumes, not just reserved for the finest or most costly compositions.

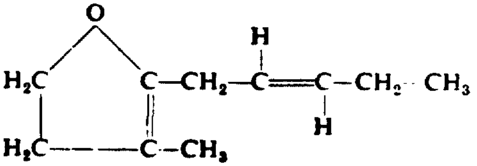
Various effects can be achieved with various types of *iso*-Jasmone: floral, fruity, minty, warm, diffusive, "lifting", oily, etc. but with respect to Jasmine similarity, they are all inferior to *cis*-Jasmone.

Prod.: (many methods), e. g. from Undecylenic acid, via Undecalactone with poly-Phosphoric acid is obtained a mixture rich in the isomer having the double bond in the side-chain, while Phosphoric acid gives a mixture of almost even amounts of the ring-unsaturated and the side-chain unsaturated component.

See also: 156-223;

## 1790: trans-JASMONE

Jasmone (synthetic),
*3*-Methyl-*2*-(*trans*-*2*-pentenyl)-*2*-cyclopenten-*1*-one.



$C_{11}H_{16}O = 164.25$

Pale yellowish or pale straw-colored oily liquid. The color increases upon ageing or exposure to daylight and air.

B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Diffusive, sweet-fatty, somewhat floral and slightly oily-fruity odor of good tenacity. The odor is less floral and more fatty than that of the *cis*-isomer. The overall impression is that this material does not reproduce very closely the tonalities of Jasmin as presented by the *cis*-isomer.

In the early days of manufacturing synthetic Jasmone, this isomer was normally present in the commercial product. The quality of the Jasmone would at times depend upon the ratio of the two isomers in the synthetic material.

Newer methods virtually avoid the production of the *trans*-isomer, and the only interest this isomer would have today is that of being an intermediate in the making of Dihydrojasmone. The latter can, however, be synthesized by ways omitting the step of Jasmone, and one can justly assume that *trans*-Jasmone may slowly become obsolete in the perfume laboratory and that it will have only academic interest.

Prod.: The synthesis from *trans-3*-Hexenol has no practical or commercial interest.

89-365; 156-223;

# Perfume and Flavor Chemicals

## (Aroma Chemicals)

## II

*By*

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For pioneering the first college programs in perfumery, flavor technique, essential oils and raw materials through the University Extension Division and The College of Pharmacy.

# Perfume and Flavor Chemicals

## (Aroma Chemicals)

VOLUME TWO

Monographs No. 1791 to 3102

(Letters K through Z)

Tables of aroma chemicals, classified in basic groups of odor and flavor types, according to unquestionable affect or structural relationship.

Tables of Odors and Flavors, classified in Basic Groups .......... I

Explanations to Index .......... VI

Radical synonyms and Index .......... VIII

Literature references

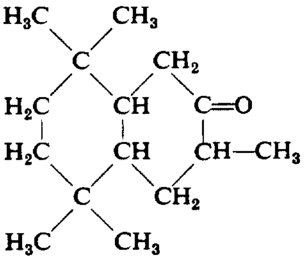
# 1791: KETONE BD-9*)

*4,7,7,10,10*-Pentamethyl-(*4,4,0*)-bicyclodecan-*3*-one.

Octahydro-*3,5,5,8,8*-pentamethyl-*2*-(*1-H*)-naphtalenone.

*) A trade name for a material produced by the U.O.P.Chemical Co., Division of Universal Products, Inc., Des Plaines, Ill. U.S.A.

The commercial product consists of at least 3 stereoisomers:



$C_{15}H_{26}O = 222.37$

Colorless or translucent crystalline mass or colorless, slightly viscous liquid forming crystals in the cold. Sp.Gr. 0.96. B.P. 290° C.

Insoluble in water, soluble in alcohol, perfume oils and mineral oil.

Pleasant, dry-woody, Ambre-like and somewhat Orris-like odor of great tenacity and remarkable odor uniformity. In spite of the distinctly dry note, there is a sweetness accompanying the wood odor, changing it to a pleasant unit with good resemblance to portions of the Ambergris picture.

This ketone, entirely a synthetic development and apparently not related chemically to a natural product, was brought on the American market in 1960 and has been used in soap perfumes and various cosmetic perfumes ever since. Its solid stability in soap and its performance apparently undisturbed by the influence of air and other normally detrimental factors have been its major assets besides of the Ambre-like character.

It blends excellently with the Ionones and particularly with the Methylionones, Cedarwood derivatives, Vetiver products, alifatic aldehydes, Cyclamal, Sandalwood, Oakmoss, etc. It forms an interesting base for ever-popular versions of the "Miss Dior" theme with Oakmoss, Galbanum and other dry, green or woody materials, also with Labdanum, many Carbinols, etc.

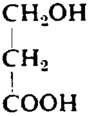
Prod.: from *2,5*-Dichloro-*2,5*-dimethylhexane plus Phenol in a Friedel-Craft's reaction. Then hydrogenation to the alcohol followed by oxidation to the ketone (isomer mixture).

Almost identical isomer mixtures are manufactured by other perfume chemical producers.

(See also The Trubek Laboratories, data sheet 1960: Ketone BD-9.). (Now: U.O.P. Cemical Co., Div. of Univ. Oil. Prod. Inc.).

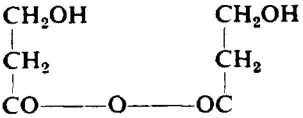
## 1792: LACTIC ACID

DL-Lactic caid (racemic Lactic acid).
2-Hydroxypropionic acid.
*alpha*-Hydroxypropionic acid.
NOTE: Commercial grade contains normally from 10 to 15% of Lactic anhydride.



$$\begin{array}{l} CH_2OH \\ | \\ CH_2 \\ | \\ COOH \end{array}$$

Lactic acid: $C_3H_6O_3 = 90.08$.



$$\begin{array}{lcl} CH_2OH & & CH_2OH \\ | & & | \\ CH_2 & & CH_2 \\ | & & | \\ CO & —O— & OC \end{array}$$

Lactic anhydride.

Colorless viscous or syrupy liquid. Miscible with water, Propylene glycol, Glycerin, Alcohol and many oils. Sp.Gr. 1.21 Decomposes when heated above 125° C. at atmospheric pressure.

Chemically pure Lactic acid is odorless, but commercial grades have a faint odor reminiscent of Buttermilk (a "reverse" odor description but probably the closest and most common one). The taste is pleasantly acid in proper dilution. It should be kept in mind that Lactic acid when undiluted is corrosive to human skin, and dissolves many types of organic tissue.

The acid is, to the author's knowledge, not used in perfume compositions.

It finds extensive use in flavors, partly as a component in certain imitation flavors: Butter, Buttermilk, Butterscotch, Milk, Cheese, Chocolate, Blackberry, Walnut, and in spice blends, fruit complexes, etc.

It is furthermore used as an acidifier in functional products such as carbonated beverages, desserts, sherbets, candy, etc. Concentration may vary from 10 to 100 ppm in ordinary finished products, 300 to 600 ppm in chewing gum, up to 8000 ppm in soft drinks and from 1000 to 25.000 ppm in pickled products.

G.R.A.S. F.E.M.A. No.2611.

Prod.: (many methods) e. g. by high temperature bacterial fermentation of Corn starch, Molasses, Whey or similar products.

26-590; 66-785; 77-190; 77-242; 100-593; B-III-268;

## 1793: LACTOSE

Milk Sugar.
*alpha*-Lactose monohydrate (commercial product).
Lactobiose.
4-(*beta*-*D*-Galactopyranosido)-*D*-glucose.

(anhydrous) $C_{12}H_{22}O_{11} = 342.31$
(monohydrate) $C_{12}H_{24}O_{12} = 360.32$

Rhomboid white crystals. Monohydrate melts at 202° C. Anhydrous material melts at 252° C. Decomposes before boiling.

Soluble 17% in cold water, 40% in hot water. Very poorly soluble in alcohol, insoluble in most oils.

Virtually odorless when pure, or of good commercial grade.

Mildly sweet taste. A typical feature is the "sandy" or "gritty" feel on the tongue, caused by the slow dissolving of Lactose.

Lactose is used as a natural "filler" in powdered flavors, extracts, food powder mixes, etc.

Its relative sweetness has been estimated at 15 to 20% of the sweetness of cane sugar, calculated at normal use concentrations. Lactose is the poorest sweetener of the common sugars related to saccharose. This low sweetness has certain advantages in these times of great concern for caloric intaking. Lactose can be used as a "carrier" for non-nutritive sweeteners and supply the missing "body" of flavor feel often encountered when artificial sweeteners are used alone. It is also easier to compress into tablet form than most other sugars.

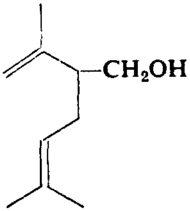
Prod.:
1) as a by-product in the manufacture of Cheese.
2) by evaporation of whey.

G.R.A.S.

26-590; 66-1296; 100-594; 160-1076; B-XXXI-407; 30-141;

## 1794: LAVANDULOL

*2-iso*-Propenyl-*5*-methylhexen-*4*-ol-*1*.
*2,6*-Dimethylmethylol-*5*-heptadiene-*2,6*.
*2,6*-Dimethyl-*5*-hydroxymethyl heptadiene-*2,6*.
An isomer of Geraniol.



$C_{10}H_{18}O = 154.25$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 203° C.

Very slightly soluble in water, soluble in alcohol and oils.

Oily-herbaceous, warm-rosy odor reminiscent of Geraniol and with a slightly spicy note. There are notes resembling those found in Cumin alcohol.

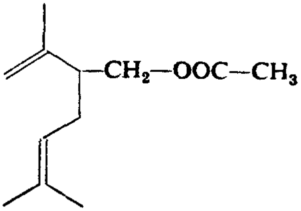
This alcohol, only recently brought into the market at a truly attractive price, has found use in artificial Lavender oils, Lavandin, Bergamot, Clary Sage, etc. As a perfume material, it has not yet found much use, perhaps because of its price was always too high for its odor type, except in the case of the specific application in artificial essential oils.

Prod.:
1) from Isoprene hydrobromide plus Sodium *iso*-propylidene malonic ester via Lavandulic acid.
2) from Methylheptenone plus Formaldehyde in a Prins' reaction followed by a Methyl Grignard reaction or a pyrolysis.

34-578; 86-83; 87-575; 65-177; 105-656; 105-672;

## 1795: LAVANDULYL ACETATE

(See also Lavandulol).



$C_{12}H_{20}O_2 = 196.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet, fruity-herbaceous and slightly warm to spicy odor of some resemblance to the odor of Linalyl propionate.

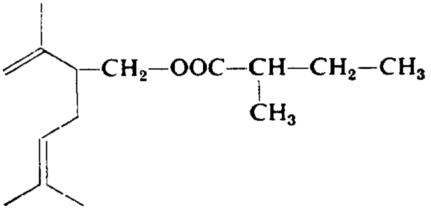
This ester finds some use in perfumery in the re-construction of various essential oils, and as a support to Bergamot- or Clarysage-type odors. It is frequently used in artificial Lavandin, Lavender and Bergamot.

The ester could find use in flavor compositions. The author finds it useful in imitation Pear and Plum, and good as a modifier in Berry flavors.

Prod.: by Acetylation of Lavandulol.

## 1796: dl-**LAVANDULYL**-alpha-**METHYLBUTYRATE**

(See also Lavandulol).



$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid. Sp.Gr. 0.90. B.P. 242° C.

Insoluble in water, soluble in alcohol and oils.

Very sweet, warm-herbaceous, Tea-like and Clary-Sage-like odor of good tenacity. Slightly fruity, fruit-preserve-like undertones.

This ester, of which the optically active isomer has been identified in Lavandin oil, has found some use in the reconstruction of Lavandin oil and a few other essential oils.

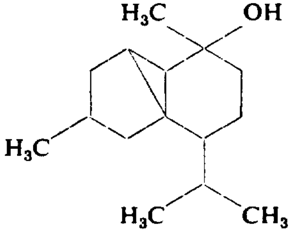
Until the ester is available at a much lower cost, there is not a great chance that it will find wide application in perfumery. It could be used in artificial Clary Sage, and if it were sufficiently inexpensive, it could be used as a modifier for Bergamot, Clary Sage and other herbaceous oils in new types of Men's fragrances, etc.

Prod.: by direct esterification – or from *d-alpha*-Methylbutyrylchloride plus *l*-Lavandulol in Benzene with a Pyridine or Dimethylaniline type catalyst.

90-277 (describes the optically active form). (Sample: Takasago Perfumery Co., Ltd.).

## 1797: LEDOL

"Ledum camphor".



$C_{15}H_{26}O = 222.37$

Colorless or white long needles or prismatic crystals. M.P. 105° C. (sublimes below melting point). B.P. 292° C. Sp.Gr. 0.91 (liquid)

Insoluble in water, Approximately 10% soluble in alcohol, soluble in most oils.

Warm and mild, pleasant odor, balsamic-sweet, slightly woody and very tenacious.

This tertiary alcohol has been suggested for use in perfume compositions as a modifier for Patchouli-Cedarwood-Sandalwood notes in non-floral or Ambre-type fragrances. It blends well with Oakmoss, Ionones, Olibanum and Galbanum, the herbaceous oils and the woody oils, with many Carbinols, Salicylates, etc.

Its availability is still limited to the very occasional production of essential oil from a comparatively rare plant.

The essential oil and the Ledol in particular have been classified as moderately toxic.

Prod.: by isolation from the higher boiling fractions of the essential oil of the Tundra Tea (Ledum palustre) a common and decorative plant in Greenland, Siberia and similar areas.

65-280; 67-676; 88-314; 100-606;

## 1798: LEVULINIC ACID

Laevulic acid.
Acetopropionic acid.
*4*-Oxovaleric acid.
*gamma*-Oxovaleric acid.
*gamma*-Oxopentanoic acid.
*3*-Acetyl propionic acid.
*gamma*-Ketovaleric acid.
*3*-Ketobutane-*1*-carboxylic acid.

$CH_3CO—CH_2—CH_2—COOH$

$C_5H_8O_3 = 116.12$

Colorless leafy crystals when pure, yellowish crystals when commercial grade. Soluble in water, alcohol, Propylene glycol, Glycerin and most oils. Darkens when exposed to sunlight. M.P. 37° C. (pure) or 34° C. (commercial grade). B.P. 246° C. under slight decomposition. Sp.Gr. 1.14 (liquid).

Mild caramellic odor, or almost odorless (when pure). Decomposition causes acid odor and pungency.

Pleasant, acid taste in proper dilution. The acidulous taste is accompanied by a caramellic flavor giving the impression of sweetness with the acidity.

This material is not used in perfume compositions.

It finds extensive use in flavors, partly as a component of various Berry-type flavor compositions, Butter, Maple and Nut imitations, Caramel and various fruit flavors, etc.

The concentration used is normally about 5 to 50 ppm in the finished product.

The acid is also used as an acid modifier in soft drinks, sherbets, desserts, etc.

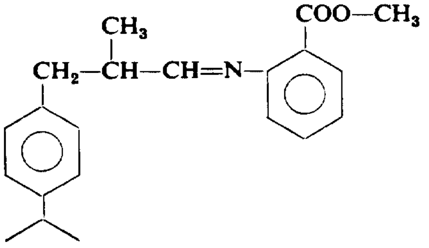
Prod.: from cane sugar or starch by mineral acid hydrolysis. Also produced from low-grade cellulose, best grades from Fructose.

G.R.A.S. F.E.M.A. No.2627.

26-592; 66-880; 100-608; 160-1078; B-III-671;

## 1799: LILIAL-METHYLANTHRANILATE

Methyl-*N*-(*para*-*tertiary*-butyl-*alpha*-methyl-hydrocinnamylidene) anthranilate.
Verdanthiol (Givaudan).
Lilianthol.
Bucinal-methylanthranilate, Schiff's Base.



$C_{22}H_{27}NO_2 = 337.47$

Intensely yellow, at times greenish-yellow, viscous liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Sweet floral and very tenacious odor with Lily-Lindenblossom character and Orange-blossom undertones. There may be variations in this odor picture according to the ratio of components used in the preparation of this material.

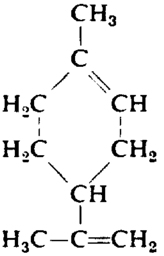
Used in perfume compositions as a modifier for "Aurantiol", the most common Schiff's base, and as a tenacious, floral note in the more delicate flower types, such as Sweet Pea, Lindenblossom, Frangipanni and in Neroli and Orangeblossom.

Prod.: by condensation of *para-tertiary*-Butyl-*alpha*-methyl hydrocinnamic aldehyde with Methylanthranilate. If preparations are made with purchased lots of the aldehyde, it must be remembered that this aldehyde is marketed with a stabilizer, so that a considerable portion of the "molecule" is non-aldehydic. It will be necessary to use an apparent surplus of the aldehyde to achieve a balanced Schiff's base.

106-343;

## 1800: d-LIMONENE

*dextro*-Limonene.
*d-para*-Mentha-*1*,*8*-diene.
*1*-Methyl-*para-iso*-propenyl-*1*-cyclohexene.
Cajeputene.
Cinene.
Carvene.
Citrene.
Hesperidene.
Kautschin.



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.84.
B.P. 177° C.

Insoluble in water, soluble in alcohol, miscible with oils, but poorly soluble in Propylene glycol, almost insoluble in Glycerin.

Fresh, light and sweet citrusy odor with strong resemblance to Orange peel oil. Commercial grade *d*-Limonene may be redistilled "Citrus Terpenes" and will then carry more Orange-like odor than a highly purified Limonene. Poor tenacity.

The taste is sweet, refreshing, Citrus-like, Orange-like, mild.

This hydrocarbon is used very extensively in perfume compositions as a refreshing top-note, particularly in the large-volume type of fragrances for household products, where the Citrus-odor is desirable or at least compatible with the product and the purpose. It may give lift without giving a true Orange character, and it can therefore be used in a multitude of fragrance types, including floral types from Jasmin to Lavender "bouquets", and in Pine, aldehydic, woody, fruity or green odors. In detergent perfumes it is often found together with Benzyl acetate. It has the added advantage of being colorless. It is often annoying to introduce an intensive yellow or orange color when cold-pressed sweet Orange oil is used in Citrus fragrances. This color may often fade away after a few months in the perfume composition and cause variations in the color of the perfume, not always understood by the customer.

It is one of the most inexpensive perfume materials, yet not necessarily confined to "cheap" fragrances. Its main drawback is that of tendency to oxidize, but this can be combated with Antioxidants which retard the oxidation to a considerable degree. Combination antioxidants of Butylhydroxyanisole, Butyl hydroxytoluene and Citric acid as a synergist are effective at concentrations far below perceptible level and may prolong the life of odor-acceptable Monoterpenes from a few months up to more than one year under same conditions of storage.

*d*-Limonene is also used in flavor compositions, mainly as a modifier in Lime, fruit and spice complexes. The pungency often encountered when using large amounts of cold-pressed Orange oil in chewing gum can be reduced by the use of *d*-Limonene based upon the theory that the pungent or "biting" components are present mainly in the non-volatile portion of the oil, therefore absent in *d*-Limonene which is a distilled product. Similar conclusions have been made on the subject of Bergamot oil in the discussion of its hazard as a possible skin-sensitizer.

The concentration of *d*-Limonene in the finished products is normally about 30 to 400 ppm, except in chewing gum where it may be as high as 2300 ppm.

Prod.: by redistillation of "Citrus oil" obtained from sweet Orange and Grapefruit in the juice processing.

G.R.A.S. F.E.M.A. No.2633.

4-81; 17-102; 26-592; 65-22; 85-78; 86-83; 87-45; 160-1078; B-V-133;
*l*-Limonene: see next monograph.
*dl*-Limonene: see Dipentene.

## 1801: l-LIMONENE

(Structure formula: see *d*-Limonene).

$C_{10}H_{16} = 136.24$

Colorless mobile liquid. B.P. 177° C.
Sp.Gr. 0.84.

Insoluble in water, soluble in alcohol, miscible with most oils.

Until recently, this modification of Limonene was not commercially available in sizeable quantities.

It is comparatively rare in Nature, and generally confined to a few Natural Orders. Certain uncommon Pine species, Carrot seed oil, a great number of oils from Labiatae (Mint oils, etc.) etc. are rich in *l*-Limonene, but the isolation of this Terpene from the named essential oils is generally not economically feasible.

Recent interest in the reconstruction of Peppermint and Spearmint oils, particularly during the very high prices in 1965-66 for Spearmint oil, encouraged the research on the subject of manufacturing *l*-Limonene.

To the author's knowledge, there is no extensive use of *l*-Limonene except in the making of artificial Mint oils and similar products.

*l*-Limonene has a refreshing, light, very clean odor, not reminiscent of Citrus fruits in particular, and not recalling any specific Pine or Mint. This could be due to the fact that the samples of *l*-Limonene available have been of purely synthetic origin.

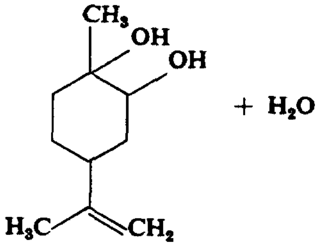
Prod.:

1) by purification of isolated Monoterpenes from certain Pine (needle) oils. Particularly silver fir cone oil.
2) *l*-Limonene has also been prepared synthetically from pinene by acid catalysis in presence of Amides to reduce the formation of Bornyl – and Fenchyl esters.

87-45;
(Glidden data, 1967).
*dl*-Limonene: see Dipentene.
*d*-Limonene: see previous monograph.

## 1802: LIMONENE DIOL

Limonene glycol.
*para*-Menthene-*8*(*9*)-diol-*1,2*.



$C_{10}H_{18}O_2 + H_2O = 188.27$
$C_{10}H_{18}O_2 = 170.25$

Colorless or opaque crystalline mass or granular crystals.
M.P. 60° C. or 73° C. (anhydrous material).

Very faint, sweet-balsamic-herbaceous odor of good tenacity.

The title material, which is rarely offered commercially, is used in perfume compositions as a blender with moderate fixative effect. It is inexpensive, relatively stable and offers a reasonable background for Citrus compositions, etc.

Glycols from commonly available Monoterpenes have been manufactured for many years, but never achieved much interest among perfumers. Various so-called glycols, including "Terpinyl glycol" are still used, but are usually perfume compositions with no relationship to the Monoterpene glycols.

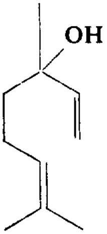
The glycol from Carene, isolated from East Indian Turpentine oil has been offered as a perfume material recently, but not yet become a regularly available item.

Prod.: by Autoxidation of Limonene. The process also yields Carveol and Carvone.

87-69;

## 1803: LINALOOL

*3*,*7*-Dimethyl-*1*,*6*-octadien-*3*-ol.
"Licareol" (*l*-Linalool from Bois de Rose oil).
"Coriandrol" (*d*-Linalool from Coriander oil).
*dl*-Linalool (synthetic Linalool).



$C_{10}H_{18}O = 154.25$

Colorless liquid. Sp.Gr. 0.86. B.P. 198° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils. Almost insoluble in Glycerin.

Light and refreshing, floral-woody odor with a faintly citrusy note. The odor description of to-day (1968) would naturally be somewhat different from descriptions prior to 1957, when pure, synthetic Linalool was an uncommon item on the perfumer's shelf. Commercial grade, synthetic Linalool does have trace impurities, and they do have an influence upon the odor of the product.

However, synthetic Linalool is – after a surprisingly hard ten-year fight – completely accepted as "Linalool" by the perfumer today. It is also interesting to note, that while synthetic Linalool has grown beyond the million-pound-a-year mark in ten years, there has been only a slight decrease in the world production of Bois de Rose oil. Part of the explanation lies in the fact that enormous amounts of Linalool (and its Acetate) are used in the making of artificial Bergamot, Lavender, Lavandin and other essential oils of which the consumption runs into very large volume figures. Thus, the synthetic Linalool has missions other than that of replacing Bois de Rose oil.

Linalool is used very extensively in perfume compositions of almost all types and price levels. Basically a floral material, and originally a Lily-of-the Valley (Muguet) ingredient, it is now used in countless floral types, and in Oriental, Ambre, aldehydic, herbaceous and many other fragrance types. It may even form part of a Citrus fragrance or a woody complex, a Lily, Muguet, Honeysuckle, Lilac, Sweet Pea, Neroli, Appleblossom, Frangipanni, Freesia, Peony, etc. etc.

Linalool is – in perfumery terms – a low-boiling ingredient, and its tenacity is notoriously poor. It requires very good and skilled fixation to utilize larger amounts of Linalool in a fragrance without having the Linalool dominating the perfume. In fact, the Linalool should be the ingredient that gives the lift in an overall heavier composition.

Newer derivatives, particularly the higher homologues of Linalool, are excellent modifiers/blenders with proper mellowing effect upon the more volatile Linalool.

Linalool has a peculiar creamy-floral, but not distinctly sweet taste. The flavor picture seems to vary considerably with the concentration. Linalool is pleasant only in low concentrations and in combination with other flavorants.

It is used frequently in Blueberry imitation, Lemon, Lime, Orange, Grape and Cola compositions, in Apricot, Pineapple Date, Blackcurrant Plum, Peach, Cardamon and other fruit and spice complexes, in meat flavors and in Cocoa and Chocolate imitation. The latter application is particularly interesting since Linalool gives very pleasant effects with Vanillin. The Vanillin seems to emphasize the creamy notes of Linalool and cover the woody notes.

Concentrations are about 2 to 10 ppm in candy, beverages, baked goods, etc. but it may be as high as 40 ppm in meat products.

G.R.A.S. F.E.M.A. No.2635.

Prod.:

1) by isolation from Bois de Rose oil. The Linalool fraction may be further purified by boration.
   Linalool from Lavandin oil and from Bergamot oil were commercial products only 10 or 15 years ago. At that time Linalool was sold at a price almost equal to that of Bergamot oil, and adulteration of Bergamot oil with Linalool "ex Bois de Rose oil" was out of the question. A product called "Saponified Paraguay Petitgrain Oil" is available from time to time. It consists mainly of Linalool (from a chemical point of view).
2) many synthetic methods, e. g.: from Acetone plus Acetylene via Methylbutynol to Methylbutenol. Then reaction with Diketene and Sodium acetylide in liquid Ammonia to produce Dehydrolinalool which is the key to Linalool and its esters.
3) by hydration of Myrcene with Acetic acid is obtained a mixture of Linalool and Linalylacetate. The mixture can find use as such in artificial essential oils, or it may be separated.

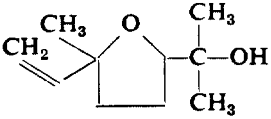
4-81; 5-22; 26-592; 31-19; 85-79; 86-83; 87-510; 77-173; 100-609; 103-224; 106-218; 160-1080; 156-233; B-I-461;

## 1804: LINALOOL OXIDE

Epoxylinalool.

"Epoxydihydrolinalool".

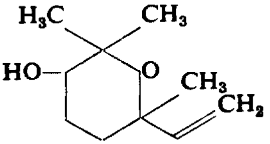
*2*-Methyl-*2*-vinyl-*5*-hydroxy-*iso*-propyl tetrahydrofuran.



A:

*2*-Hydroxy-*2,6*-dimethyl-*3,6*-epoxyocten-*7*.

*2*-Hydroxy-*iso*-propyl-*5*-methyl-*5*-vinyltetrahydrofuran.



B:

Tetrahydro-*2,2,6*-trimethyl-*6*-vinylpyran-*3*-ol.

$C_{10}H_{18}O_2 = 170.25$

Formula B was preferred until 1963, when the formula A was repeatedly established as the correct formula of the chief component of Linalool oxide.

Colorless, slightly oily liquid. B.P. 188° C. Sp.Gr. 0.94.

Powerful sweet-woody, penetrating odor with floral-woody-earthy undertones. Undiluted almost pungent, it reveals more pleasant floral woody character upon dilution. The camphoraceous notes bear some resemblance to those of Cineole (Eucalyptol).

This oxide finds some use in perfumery, partly as a component in artificial essential oils (Lavandin, Geranium, Lavender, etc.), partly as a powerful additive to Lavender-Lavandin type fragrances.

It has also been used to create "natural" notes in Linalool since the presence of Linalool oxide in Natural Linalool was confirmed and believed to be of importance.

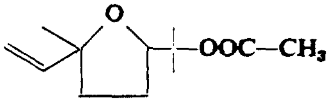
It is now mostly used for its power in soap perfume with Lavandin and Spike Lavender oils.

Prod.: from Linalool by oxidation.

90-731; 156-238;

## 1805: LINALOOL OXIDE ACETATE

"Epoxylinalyl acetate".
Linalyl acetate epoxide.



$C_{12}H_{20}O_3 = 212.29$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

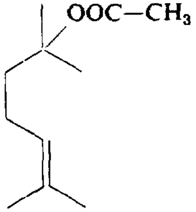
Soft and sweet fresh and floral odor with an overall "natural" note. It is somewhat more woody than the acetate, not as "candy-like".

The ester finds some use in artificial Lavandin and Lavender bases.

90-731; (see also Linalool oxide).
(Sample: Hoffmann-laRoche, Inc.).

## 1806: LINALYL ACETATE

*3*,*7*-Dimethyl-*1*,*6*-octadien-*3*-yl acetate.



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. Sp.Gr. 0.91. B.P. 220° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils. Insoluble in Glycerin.

Sweet, floral-fruity odor recalling Bergamot and Pear. The tenacity is moderate to poor. Synthetic Linalylacetate displays an overall "cleaner", less complex odor than the Acetates produced from natural Linalool (from Bois de Rose oil, Ho leaf oil, etc.).

This ester is very widely used in perfume compositions as a fresh and sweet modifier/blender, as an additive to compositions rich in Bergamot, Lavender, Lavandin, Petitgrain, etc. and in fruity topnote complexes, etc. With esters of Citronellol and Geraniol it may emphasize the effect of Bergamot oil, or it supports the fresh notes of Citrus oils.

The ester does not perform very well in soap unless very solidly fixed and it is quite sensitive to mild acid or mild alkali in presence of moisture.

The taste is sweet, fruity, Pear-like with a faintly floral note. It finds some use in flavor compositions for Berry complexes, Citrus flavors, Pineapple, Gooseberry, Peach or Pear imitations, Ginger spice blends, etc. The concentration is normally about 2 to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2636.

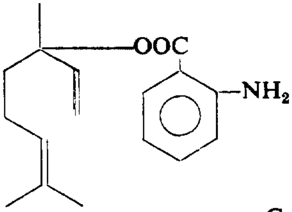
Prod.: from Linalool by esterification, using various methods for protection of the tertiary alcohol in the acid mixture. Newer methods are based upon esterification of Dehydrolinalool followed by hydrogenation of Dehydrolinalyl acetate, thus avoiding above problem.

Linalyl acetate is also prepared by a number of methods starting from Myrcene via Linalyl chloride.

33-503; 90-247; 100-609; 106-221; 160-1080; 156-245; B-II-141; 26-592; 77-183; 103-97; 4-82; 86-83; 5-247; 85-79; 95-177; 96-211;

## 1807: LINALYL ANTHRANILATE

Linalyl-*ortho*-aminobenzoate.



$C_{17}H_{23}NO_2 = 273.38$

Pale straw-colored or almost colorless oily liquid. B.P. over 320° C. Sp.Gr. 1.06.

Almost insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol.

Soft-floral and very tenacious Lindenblossom-Acacia-Neroli type odor.

Sweet, floral-fruity and comparatively powerful taste with a variety of green, fruity, Grape-like, berry-like notes, according to origin of sample.

This ester, not often offered commercially, finds a little use in perfumery as a modifier in Orangeblossom, Neroli, Lilac, Sweet Pea, Wistaria, Freesia, Frangipanni and other fragrance types.

It is also used in flavor compositions in trace amounts in imitation Grape, Pineapple and in Citrus complexes, berry and fruit flavors, etc. The concentration in the finished product will normally be as low as 0.2 to 5 ppm.

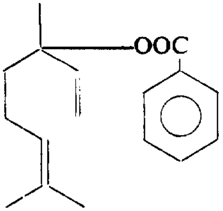
G.R.A.S. F.E.M.A. No.2637.

Prod.:

1) from Linalyl formate plus Methylanthranilate with Sodium Linalool.
2) from Linalool plus Isatoic anhydride with trace of Sodium hydroxide as starter catalyst.

4-82; 34-1022; 103-165; 156-43;

## 1808: LINALYL BENZOATE



$C_{17}H_{22}O_2 = 258.36$

Almost colorless oily liquid. Sp.Gr. 0.99 B.P. 263° C.

Insoluble in water, soluble in alcohol and oils.

Balsamic-floral, Bergamot-fruity odor of good tenacity. The odor varies considerably according to the method of production of this ester. Above description is based upon the "Roche"-processed material, while older methods yield esters of far greater sweetness, less tenacity and more similarity to Linalyl acetate, often with side-notes of Methylbenzoate.

Peculiar, deep-sweet, fruity or fruit-preserve-like odor, mainly of Plum-type.

An interesting material for new variations of the conventional theme in Men's fragrances. Particularly suitable for "outdoor" type odors, Bruyere, woody-green, mossy-green or green-citrusy types. Also used in Oriental fragrances, in heavy florals such as Gardenia, Tuberose, Stephanotis, etc.

This ester finds some use in flavor compositions for imitation Peach, Plum, Blackcurrant and other berries, fruit complexes or Citrus flavors. The concentration in the finished product will normally be about 0.3 to 2 ppm.

G.R.A.S. F.E.M.A. No.2638.

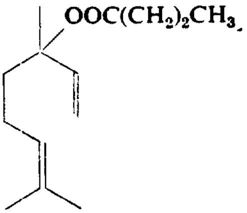
Prod.:

1) from Linalyl formate plus Methylanthranilate with Sodium Linalool.
2) by esterification of Dehydrolinalool with Benzoic acid e. g. under azeotropic conditions, followed by hydrogenation of the Dehydro-ester.
3) from Linalool sodium with Trichloro acetophenone.

4-82; 5-251; 86-83; 103-131; 106-223; 156-240;

## 1809: LINALYL BUTYRATE

Linalyl-*n*-butyrate.



$C_{14}H_{24}O_2 = 224.35$

Colorless, slightly oily liquid. Sp.Gr. 0.90. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Heavy-fruity, sweet and Bergamot-like, Pear-like odor of moderate tenacity.

Sweet-fruity, Plum-and-Honey-like taste with dry-fruity notes.

This ester finds use in perfume compositions mainly for Lavender notes in Colognes (Citrus-colognes), Fougères, and in many types of Lilac, Muguet, Cassie, Peony and other floral bases.

It is furthermore used in flavor compositions for imitation Banana, Butter, Grape, Honey, Loganberry, Melon, Peach, Pear, Pineapple, Plum, and in Caramel flavors, Citrus blends, fruit complexes, Spice blends, Nut flavors, Rose or other floral types, etc.

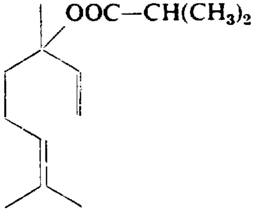
The concentration is normally low, about 0.1 up to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2639.

Prod.: from Dehydrolinalool by esterification and subsequent hydrogenation – or by esterification of Linalool with Butyric anhydride (old method).

4-82; 31-123; 33-734; 77-186; 86-83; 90-271; 103-116; 106-224;

## 1810: LINALYL-iso-BUTYRATE



$C_{14}H_{24}O_2 = 224.35$

Colorless, slightly oily liquid. Sp.Gr. 0.89. B.P. 230° C.

Insoluble in water, soluble in alcohol and oils.

More floral and less fruity than the *n*-Butyrate, not quite as "heavy" and less Plum-like. More rosy, yet overall fresh, sweet. Moderate tenacity.

Sweet, fruity taste, but rather nondescript of fruit-type. More Berry-like and less Plum-like as compared to the *n*-Butyrate.

Finds use in perfume compositions, mainly in Lavender complexes, Bergamot bases, Lilac and Citrus-colognes, etc.

The ester is also used in Banana, Black-currant, Cherry, Pear, Pineapple, Plum and other imitation fruit flavors, as well as in Nut, Spice, Citrus, Berry and various fruit complexes and bases.

Concentration varies from 2 to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2640.

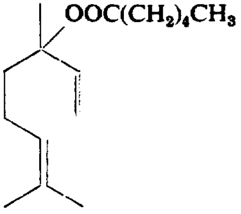
Prod.: by esterification of Dehydrolinalool, followed by hydrogenation of the Dehydrolinalyl ester.

The ester is still prepared by the older meththod from Linalool and *iso*-Butyric acid or anhydride in an inert diluent.

4-83; 33-734; 86-84; 103-117; 106-226; 156-240;

## 1811: LINALYL CAPROATE

Linalyl hexanoate.
Linalyl hexoate.



$C_{16}H_{28}O_2 = 252.40$

Colorless oily liquid. SP.Gr. 0.90.
B.P. 252° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar dry-fruity and somewhat animal odor. The term "metallic" is sometimes included in the odor description of this ester, and not infrequently met with in description of Hexyl esters and hexoates. However, the author finds that the true odor of Linalyl hexoate is primarily fruity, and that the "metallic" note – if present at all – could be due to trace impurities. The fact that the "metallic" note always disappears upon dilution tempts one to conclude so.

Thus, the flavor is mainly Pineapple-like, also Pear-like, and overall somewhat dry and reminiscent of the odor of canned fruits (pasteurized and devoid of fresh natural topnotes).

The ester is used occasionally in Lavender bases or as part of various fruity topnote compositions.

As a flavor material, its use is somewhat restricted to Pineapple imitations and variations of "Tutti-frutti" complexes.

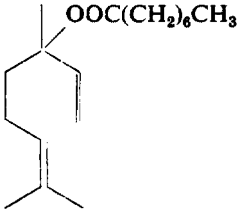
Concentrations will be around 3 to 15 ppm in the finished product.

Prod.: by esterification of Dehydrolinalool with *n*-Hexanoic acid, followed by hydrogenation of the Dehydro-ester.
G.R.A.S. F.E.M.A. No.2643.

4-82; 86-83; 90-279;

## 1812: LINALYL CAPRYLATE

Linalyl octanoate.
Linalyl octoate.



$C_{18}H_{32}O_2 = 280.45$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 264° C.

Insoluble in water, soluble in alcohol and oils.

Mild and somewhat dry-fruity, herbaceous odor of good tenacity. There is some resemblance to the odor of unripe Peaches.

Sweet, oily-fruity taste, reminiscent of Apricot and unripe Plum. The taste is accompanied by a somewhat "perfumey" note which is not always desirable in flavors.

The ester is occasionally used in Lavender, Rose and Citrus compositions in perfumery.

It is also used in Apple, Pineapple and Honey imitations, Citrus complexes and various Citrus modifications.

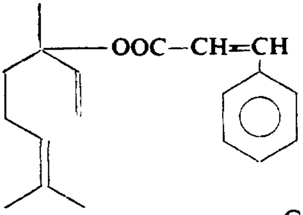
The concentration in flavored products is about 0.5 to 15 ppm.

G.R.A.S. F.E.M.A. No.2644.

Prod.: By esterification of Dehydrolinalool with Octanoic acid, followed by hydrogenation of the Dehydrolinalyl octanoate. The ester is sometimes made by esterification of Linalool with *n*-Octanoic acid under azeotropic conditions.

4-83; 90-281;

## 1813: LINALYL CINNAMATE



$C_{19}H_{24}O_2 = 284.40$

Almost colorless oily or slightly viscous liquid. Esters prepared by older methods (other than the Dehydrolinalool-route) may be straw-colored or pale amber of color.

Sp.Gr. 0.98. B.P. 353° C.

Mild and balsamic-sweet, slightly herbaceous-floral, Muguet-like, Lily-like odor of great tenacity and uniformity. Esters, prepared by methods other than the "Roche-method" may display odors largely deviating from the above description: more fruity, more complex, less floral, etc.

This ester has been used for many years in perfume compositions. However, it has not always been possible to substitute the "old type" ester with the "Roche-type" ester in an established formula, particularly in formulae where the ester enters as a major component (many delicate florals etc.). It is most conceivable that the "Roche-type" ester will supersede the very impure esters made by "older" methods.

The fixative effect and the soft fruity-herbaceous undertones produced by this ester are often utilized in delicate floral bases such as Muguet, Lily, Freesia, etc.

Trace amounts of the ester are used in flavor compositions for imitation Grape, Honey, Loganberry, and in Rose complexes, Fruit blends or Floral flavor types.

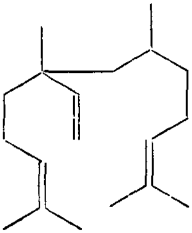
G.R.A.S. F.E.M.A. No.2641.

Prod.:

1) from Linalyl formate plus Methylcinnamate plus Linalool sodium.
2) from Dehydrolinalool and Cinnamic acid via the Dehydro-ester, which is hydrolyzed to the subject ester. ("Roche"-method).

## 1814: LINALYL CITRONELLATE

Occasionally referred to as "Linalyl rhodinate".



$C_{20}H_{36}O_2 = 308.51$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, floral odor of good tenacity.

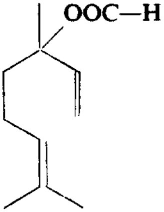
This ester is very rarely offered on a commercial basis, and the author believes that it will not achieve much more than academic interest.

If it was prepared in the attempt to achieve a product combining the best virtues of the two parent components, this aim was certainly not reached. And a major drawback is the comparatively high cost of producing this material.

4-83;

## 1815: LINALYL FORMATE

*3*,*7*-Dimethyl-*1*,*6*-octadien-*3*-yl formate.



$C_{11}H_{18}O_2 = 182.27$

Colorless moblile liquid. Sp.Gr. 0.92. B.P. 202° C.

Almost insoluble in water, soluble in alcohol and oils.

Very fresh citrusy, green-Bergamot-like, herbaceous Coriander odor of moderate to poor tenacity.

Sweet Apricot or Peach-like flavor, fresh, slightly spicy and green.

Useful in Citrus fragrances as a further "lift" to Bergamot or Lemon, and often used in Chypre type fragrances or aldehydic-fruity complexes. Absolute absence of water (moisture) is one of the prerequisites to keep this ester from decomposing, and it is therefore not strongly recommended for soap or cream.

It is also used in flavor compositions for imitation Pineapple, Apricot, Peach, Apple and various Berry complexes.

The concentration is normally as low as 1 to 15 ppm in the finished product.

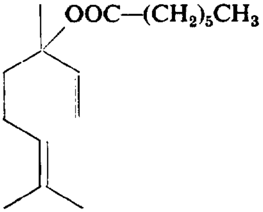
Prod.: By formylation of Dehydrolinalool, followed by hydrogenation of the ester.

G.R.A.S. F.E.M.A. No.2642.

5-251; 77-179; 103-85; 106-225; 156-240; 160-1080;

## 1816: LINALYL HEPTOATE

Linalyl heptylate.
Linalyl heptanoate.



$C_{17}H_{30}O_2 = 266.43$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Floral, slightly green, Mimosa- and Lily-like odor of good tenacity.

This ester, rarely offered commercially, finds a little use in perfume compositions, mostly in delicate floral types such as Lily, Muguet, Lilac, Mimosa, Freesia, etc.

It blends well with the "rose alcohols" in light variations of Rose or Lily, and it adds a pleasant oily greenness to the named floral types.

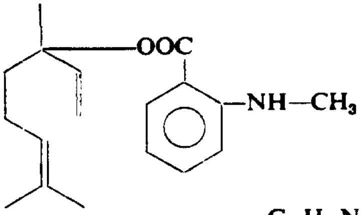
Prod.: from Dehydrolinalool and *n*-Heptanoic acid by esterification, followed by hydrogenation of the ester.

It can also be prepared by direct esterification of Linalool with *n*-Heptanoic acid under azeotropic conditions.

4-83;

## 1817: LINALYL-N-METHYLANTHRANILATE

Linalyl-2-methylaminobenzoate.



$C_{18}H_{25}NO_2 = 287.41$

Pale straw-colored viscous liquid.
Sp.Gr. 1.03. B.P. approximately 345° C.

Insoluble in water, soluble in alcohol and oils.

Sweet and very tenacious, mild but "heavy-floral" odor with balsamic-Lavender-Honeysuckle notes, sometimes with Orangeblossom character. The odor varies with the method of preparation.

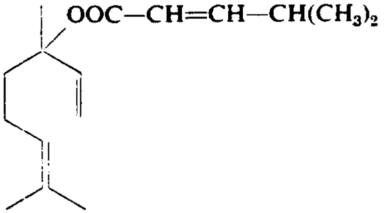
This rare ester finds some use in perfume compositions, mainly in the heavy floral or Oriental fragrance types, where tenacity is desirable. However, the general opinion is that the ester is of very little odor value and it does not offer any new or characteristic notes unobtainable with conventional materials.

Prod.: from *n*-Methylisatoic anhydride plus Linalool.

4-83; 34-1022; 86-84;

## 1818: LINALYL METHYLTIGLATE

Linalyl-4-methyl-2-pentenoate.



$C_{16}H_{26}O_2 = 250.38$

Colorless or pale straw-colored liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, powerful odor with somewhat medicinal-woody undertones and moderate tenacity.

This ester has been suggested for use in various non-floral fragrance types, also in Lavender compositions, as a modifier for Clary Sage, etc.

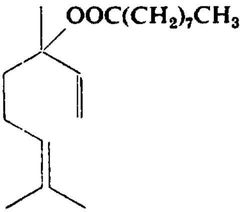
It is not regularly offered in commercial quantities.

Prod.: from Linalool and 4-Methyl-2-pentenoic acid by azeotropic esterification.

4-83;
(sample- Fairmount Chem. Co., Newark, N. J., U.S.A.).

## 1819: LINALYL PELARGONATE

Linalyl nonanoate.
Linalyl nonylate.



$C_{19}H_{34}O_2 = 294.48$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 264° C.

Insoluble in water, soluble in alcohol and oils.

Mild oily-waxy, delicately floral Rose-Lily type odor of good tenacity.

This ester has been suggested for use in perfume compositions for floral, Oriental and various fantasy fragrance types. It blends well with the Ionones and Methylionones as well as with the "rose alcohols", etc.

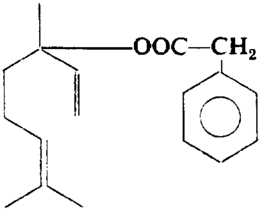
It gives interesting effects with Coumarin and traces of Nonanolide, and pleasant modifications of the winey types of topnote for delicate floral or Ambre fragrances.

Prod.: from Dehydrolinalool by esterification with Nonoic acid followed by hydrogenation of the ester, or by azeotropic esterification of Linalool with Nonoic acid.

4-83; 90-282;

## 1820: LINALYL PHENYLACETATE

Linalyl-*alpha*-toluate.



$C_{18}H_{24}O_2 = 272.39$

Colorless or pale straw-colored viscous liquid. Sp.Gr. 0.97. B.P. approximately 317° C.

Insoluble in water, soluble in alcohol and oils.

Mildly floral, intensely sweet Neroli-Rose type odor of great tenacity and with variable amounts of Honey-like undertones, according to origin of sample or method of production.

This ester, not frequently offered commercially, finds some use in perfume compositions for heavy floral types, exotic florals such as Frangipanni or Passionflower. It may form part of a fixative base for the more volatile "rose alcohols" and lighter esters in a composition, and, in turn, its own Rose-honey fragrance is brought up to life by action of the volatile components. Its tenacity is often underestimated and the material seems to grow as the perfume evaporates and leaves an increasing proportion of this ester behind. Fixation with tenacious and mild-smelling fragrance materials is necessary.

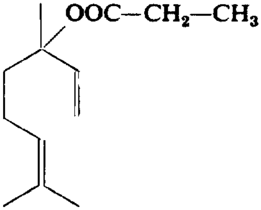
Prod.:

1) from Dehydrolinalool and Phenylacetic acid, followed by hydrogenation of the ester.
2) from Linalool sodium plus Phenylacetyl chloride.

4-83; 34-246; 86-84; 103-141;

## 1821: LINALYL PROPIONATE

*3,7*-Dimethyl-*1,6*-octadien-*3*-yl propanoate.



$C_{13}H_{22}O_2 = 210.32$

Colorless liquid. Sp.Gr. 0.90. B.P. 226° C.

Very slightly soluble in water, soluble in alcohol and oils. Slightly soluble in Propylene glycol, insoluble in Glycerin.

Fruity-floral, fresh and very sweet Bergamot-Muguet-Pear-like odor of moderate tenacity.

Sweet fruity taste, reminiscent of Pear and Pineapple.

This ester is widely used in perfume compositions, not only as a support to Bergamot-notes, but in general as a sweet fresh additive in Citrus fragrances, light florals, herbaceous types or Ambre bases. It blends excellently with Clary Sage and Bergamot for Fougère topnotes, and introduces soft sweet notes as background for the middle notes of Muguet, Lilac, Freesia and many other floral types.

The ester finds use in flavor compositions, partly as a sweetener, partly as fruity background in imitation Banana, Blackcurrant, Redcurrant, Orange, Pear, Pineapple, and in "Tutti-frutti" etc.

Concentration is normally about 3 to 12 ppm in the finished product.

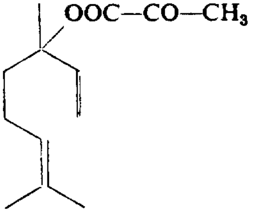
Prod.: from Dehydrolinalool and Propionic acid by esterification. The resulting Dehydrolinalyl propionate is hydrogenated to subject ester.

G.R.A.S. F.E.M.A. No.2645.
FCC-1964-851.

4-83; 31-123; 33-622; 86-84; 90-269; 103-108; 106-227; 156-240;

## 1822: LINALYL PYRUVATE

*3*,*7*-Dimethyl-*1*,*6*-octadien-*3*-yl acetylformate.
Linalyl-*2*-oxopropanoate.



$C_{13}H_{20}O_3 = 224.30$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Peculiar, sweet-herbaceous, somewhat caramellic odor with floral-herbaceous undertones and moderate tenacity.

This ester has been suggested for use in perfume compositions, but in view of the notorious instability of pyruvates in perfume compositions, their tendency to create acetic notes, one would hesitate to underwrite a recommendation for use of that ester.

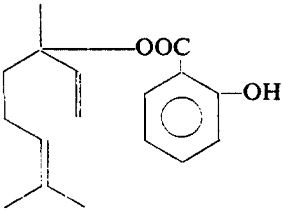
The author finds that this ester would soon be obsolete or have little more than academic interest.

Prod.: by azeotropic esterification of Linalool with Pyruvic acid.

4-83;

## 1823: LINALYL SALICYLATE

Linalyl-*ortho*-hydroxybenzoate.



$C_{17}H_{22}O_3 = 274.36$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Very mild odor, in fact it appears odorless to many observers. Musky-sweet, faintly floral or fruity odor of good tenacity.

The ester is nevertheless interesting as a fixative in mild or delicate floral fragrances such as Muguet or Lily, and blends very well with Lavender in Fougère types as a part of the fixative base.

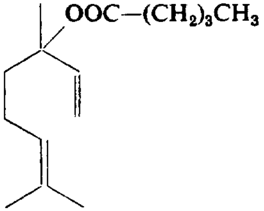
In floral fragrances, it gives a slightly green and refreshingly light but persistent background odor, very desirable in Muguet, Freesia, Narcissus, etc. This effect can be further emphasized with the more delicate carbinols or high-boiling Cinnamates, etc.

Prod.:
1) from Dehydrolinalool by esterification with Salicylic acid, followed by hydrogenation of the ester.
2) from Linalool and Salicylic acid by azeotropic esterification.
3) from Linalool and Trichloro-*ortho*-hydroxyacetophenone.

4-83; 34-758; 86-84;

## 1824: LINALYL-n-VALERATE

Linalyl-*n*-pentanoate.



$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid. Sp.Gr. 0.90.
B.P. 238° C.

Insoluble in water, soluble in alcohol and oils.

Fruity, Citrus-Lavender type odor of moderate tenacity. Overall rather heavy and not typically refreshing. More herbaceous than the lower esters.

Apple-Pineapple-like flavor in dilutions below 5 ppm.

This ester finds some use in perfumery as a modifier in Lavender fragrances, or in Bergamot odors. It gives interesting "sophisticated" effect in Pine fragrances – when cost allows for its use in that type.

In flavors, it finds use in imitation Peach, Plum, Apricot, Apple and in various types of fruit complexes.

It is not specifically mentioned in the American G.R.A.S. list, but the *iso*-Valerate is mentioned and the trade is often very lenient in using the name "Valerate" for an "*iso*-Valerate" and vice-versa.

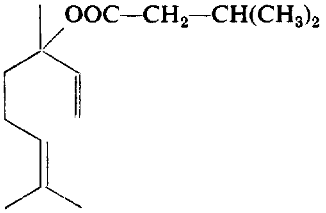
Prod.: from Dehydrolinalool by esterification with *n*-Valeric acid, followed by hydrogenation of the ester.

Also by azeotropic esterification of Linalool with *n*-Valeric acid.

4-83; 33-9-3; 5-238; 86-84; 90-275;

## 1825: LINALYL-iso-VALERATE

Linalyl-*iso*-pentanoate.



$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, fruity, citrusy odor, rich, Apple-like, Clary-Sage and Tea-like undertones and moderate tenacity.

Apple-like, sweet and powerful taste, remotely reminiscent of Peach and Plum.

This ester finds use in heavy exotic floral fragrance types, in Chypres and some Oriental types. It blends excellently with Clary Sage and Oakmoss, as well as Jasmin, Neroli and Petitgrain. It seems to be very stable and performs well in soap.

In flavor compositions, it finds its way into imitation Apple, Apricot, Loganberry and other berries, Peach, Plum, etc. in the concentration equivalent to 1 to 6 ppm in the functional consumer product.

Prod.:

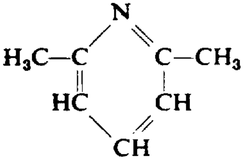
1) From Dehydrolinalool and *iso*-Valeric acid, followed by hydrogenation of the Dehydrolinalyl *iso*-valerate.
2) from Linalool and *iso*-Valeric acid by azeotropic esterification.

G.R.A.S. F.E.M.A. No.2646.

4-83; 5-238; 86-84; 90-276; 103-125;

## **1826:** alpha-alpha'-**LUTIDINE**

*2,6*-Lutidine.
*2,6*-Dimethylpyridine.



$C_7H_9N = 107.16$

Almost colorless or pale yellowish mobile liquid. Sp.Gr. 0.93. B.P. 144° C.

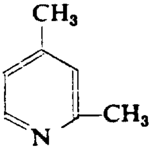
Miscible with water, soluble in alcohol, poorly soluble in oils. Pungent, yet light and nauseating-ethereal-herbaceous odor with sweet, breadlike undertones. Its topnote has been compared to the odor of human breath after Vitamin B-12-injection. Has been suggested for use in perfume compositions to introduce sweet, meat-like, "smoky" notes, e.g. in artificial Oakmoss, etc.

Prod.: by isolation from coal tar, purified over the Mercury salt, or: synthetically from Ethyl acetoacetate plus Formaldehyde plus Ammonia.

26-592; 69-524; 100-620; B-XX-244;
Sample: Reilly Tar and Chemical Co. (U.S.A.).

## **1827:** alpha-gamma-**LUTIDINE**

*2,4*-Lutidine.
*2,4*-Dimethylpyridine.



$C_7H_9N = 107.16$

Colorless liquid. Sp.Gr. 0.94. B.P. 158° C.

20% soluble in water, soluble in alcohol and most oils.

Powerful and diffusive minty-tarry odor of poor tenacity (when the material is pure, but technical grades leave a very tenacious naphthalenic dryout note).

This material has been suggested for use in perfume compositions to introduce new types of "leather-like" notes, give lift and power or support individual notes in a fragrance.

The material suffers however, from drawbacks similar to those of related chemicals: discoloration, possible skin-irritation to human skin, incompatibility with several types of perfume materials etc.

It should be kept in mind that Piperidine and other related chemicals are used and permitted in perfumes and flavors, see monograph: Piperidine.

It is most conceivable that this material will remain a very rarely used one in perfumes. It is not used in flavors, as far as the author is aware.

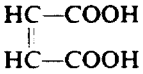
Prod.:

1) from coal tar distillates.
2) from bone tar distillates. (Bone tar oil).

1-813; 26-592; 69-524; 160-1080; B-XX-244; see also: 30-266; 30-268; 31-192;

## 1828: MALEIC ACID

*cis*-Butene dioic acid.
(Fumaric acid is the *trans*-form).
Toxilic acid.
*cis-1,2*-Ethylene dicarboxylic acid.



$$\begin{array}{l}\mathrm{HC{-}COOH}\\ \ \ \| \\ \mathrm{HC{-}COOH}\end{array}$$

$C_4H_4O_4 = 116.08$

White crystals. M.P. 130° C.

Very soluble in water and alcohol, poorly soluble in most oils.

Faintly caramellic odor.

Acid-astringent taste and mouthfeel, not exactly pleasant.

Concentrations up to 100 ppm of this acid are used in fats and oils intended for food use. The addition of this acid will retard rancidity processes in the oils.

This acid is mentioned mainly for the purpose of completing the description of the three acids with similar names: Malic acid, Maleic acid and Malonic acid. Only Malic acid has considerable interest to the flavor industry, see notes under Malonic acid.

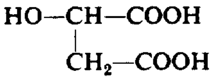
Prod.: (many methods) e. g.:

1) by heating of Malic acid.
2) from Benzene by vapor phase oxidation in presence of a Vanadium catalyst.
3) as a by-product in the preparation of Phthalic anhydride is obtained Maleic anhydride, which is transformed into the acid.

26-592; 66-990; 100-631; B-II-748;

## 1829: l-MALIC ACID

*l*-Hydroxybutane dioic acid.
*l*-Hydroxysuccinic acid.
"Apple acid" (the *laevo*-form is natural).
"Pomalus Acid", (Allied Chemical Corp.).



$$\begin{array}{l}\mathrm{HO{-}CH{-}COOH}\\ \qquad\ |\\ \qquad \mathrm{CH_2{-}COOH}\end{array}$$

$C_4H_6O_5 = 134.09$

Colorless needles. M.P. 100° C.
B.P. 140° C. (decomposes).

Soluble in water, alcohol and Propylene glycol. Slightly soluble in various perfume and flavor materials.

Odorless or having a very faint, caramellic-acrid odor.

Tart-acidulous taste with a caramellic sharpness, yet not unpleasant or pungent. Approximately 15 to 20% more efficient as an acidifier when compared to Citric acid. Also less hygroscopic.

This material is widely used in flavors, or rather in foods as an additive, acidifier or acid modifier, particularly in soft drinks, sherbets, hard candy, etc.

It is mainly used along with fruit and Maple flavors, and the concentration in the edible product is normally about 400 to 500 ppm. Highest concentrations are usually found in candy.

The acid is quite common in natural products and is found in considerable proportion in Plum, Peach, Apricot and related fruits.

G.R.A.S. F.E.M.A. No.2655.

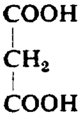
Prod.:

1) by hydration of Maleic acid, which is obtained by catalytic oxidation of Benzene vapors over Vanadium pentoxide.
2) by fermentation process from sugars.

1-282; 26-592; 77-190; 100-632; 160-1082; B-III-417;

## 1830: MALONIC ACID

Propane dioic acid.
Methane dicarboxylic acid.



$HOOC-CH_2-COOH$

$C_3H_4O_4 = 104.07$

White crystals. M.P. 136° C. (decomposes).

73% soluble in water, 35% soluble in alcohol, slightly soluble in oils.

Practically odorless. Acid, somewhat acrid-astringent taste, not very pleasant.

This acid is mentioned mainly for the purpose of completing the picture of Malonic – Maleic – Malic acids, the names of which are often confused.

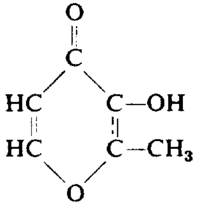
Of the three, only Malic acid has considerable interest to the flavoring industry. Maleic acid finds some use as a preservative, while Malonic is rarely used as such in flavors. Many malonic esters are used in flavor compositions and are listed in this work.

Prod.: from Sodium cyanide plus Monochloroacetic acid to Cyanoacetic acid, which is hydrolyzed to subject material.

1-282; 26-592; 66-961; B-II-566; 100-632;

## 1831: MALTOL

Palatone (Dow Chem. Co.). (Glidden Co.).
"Corps Praline" (main component) (Firmenich & Cie.).
"Mellotone" (Fritzsche Bros. Inc.).
"Veltol" (Pfizer & Co.).
Larixinic acid.
*2*-Methyl pyromeconic acid.
*3*-Hydroxy-*2*-methyl-*4*-pyrone.
*3*-Hydroxy-*2*-methyl-(*1*,*4*-pyran).
*3*,*4*-Dioxo-*2*-methyl-(*1*,*4*-pyran)-dihydride.
*3*,*4*-Dioxo-*2*-methyl-*2*,*3*-dihydro-*1*,*4*-pyran.
*3*-Hydroxy-*2*-methyl-*gamma*-pyrone.
Laricin.
– and many other trade names.



$C_6H_6O_3 = 126.11$

White crystals, volatile with steam.
M.P. 164° C.

Solubility at room temperature:
1.2% in water,
1.2% in Glycerine,
2.8% in Propylene glycol,
3.3% in Ethyl alcohol,
5.0% in Phenylethyl alcohol,
very poorly soluble in Terpenes and most other hydrocarbons. The material sublimes at 93°C. and its vapor pressure at room temperature is relatively high. Accordingly, the material evaporates rapidly unless kept in tightly closed container.

Warm-fruity, caramellic-sweet odor with emphasis on the caramellic note in the dry state, while solutions of Maltol show a pronounced fruity, jam-like odor of Pineapple, Strawberry type. Glycol-solutions show more Strawberry-like character, and Phenylethylalcohol-solutions of Maltol are more balsamic, Pine-like, with fruity undertones. The tenacity is excellent in spite of the unusually high vapor pressure at room temperature.

Intensely sweet, fruity, jam-like, Pineapple-Strawberry type flavor with caramellic undertone. The caramellic effect is predominant at high (20 to 100 ppm) concentrations, while the fruity effect is most attractive at much lower concentrations. The flavor is furthermore strongly dependent upon the presence of Vanillin, Heliotropine and other flavor sweeteners, some of which act as enhancers upon Maltol.

Maltol is commonly used in perfume compositions, but only in very low concentrations.

Its effect in Pine Needle type fragrances is well known and widely used, and its warm-sweetening effect in Rose undertones is also highly appreciated. As a trace component in fruity lipstick fragrances, often with Undecanolide, Ethylmethylphenylglycidate, Ionones, etc. it finds extensive use.

Its main use is, however, in flavor compositions, not only as fruity component in Pineapple and Strawberry, but in general as a sweetener. Its flavor is clearly perceptible at concentrations near 5 ppm, and the concentration in finished products is normally about

5 to 25 ppm in beverages
40 to 170 ppm in marmelades
100 to 200 ppm in concentrated soups
50 to 250 ppm as a general flavor enhancer.

For "bouquetting" e. g. in dentifrice flavors, minute amounts will suffice, normally equivalent to a few ppm.

An interesting feature of Maltol is its effect as a fungus growth inhibitor at concentrations of 0.1 % (however, the finished consumer product will never contain such high concentration of Maltol).

It is widely distributed in Nature and it has been manufactured since late in the 19th century. Only the last few decades have brought the material into commercial production and reasonable price level.

Maltol is unstable in alkaline media, and it discolors in presence of Iron, under influence of air and daylight, but it is quite stable in mild acids. Its vapors are capable of penetrating plastic bags, and if Maltol is stored in plastic bags inside a cardboard or fibre drum which has nails or wirestaples in it, discoloration will appear quickly and very conspicuously near the traces of metal.

G.R.A.S. F.E.M.A. No.2656.

Prod.:

1) (biosynthesis): by alkaline hydrolysis of Streptomycin salts.
2) (chemical synthesis): from Pyridine via Piperidine to Pyromeconic acid. The *2*-Methyl-derivative is Maltol.

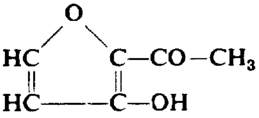
1-809; 4-110; 69-829; 100-632; 104-249; 70-101; 155-112; 156-373; 157-470ff.; 158-165; 159-661; 163-354;
see also: Chas. Pfizer Co. data sheet No.568 ("Veltol") May 1966 – and: monograph: *iso*-Maltol – and: monograph: *3*-Hydroxy-*2*-ethyl-*gamma*-pyrone.

## 1832: iso-**MALTOL**

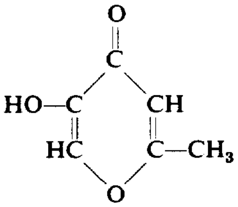
*2*-Acetyl-*3*-hydroxyfuran.
*3*-Hydroxy-*2*-furylmethylketone.

NOTE: This material is occasionally confused with Allo-maltol, which is *5*-Hydroxy-*2*-methyl-*gamma*-pyrone.

Structures of the two materials are given below.



*iso*-Maltol



Allo-Maltol

$C_6H_6O_3 = 126.11$

White crystalline powder or granular crystals.

Slightly soluble in water, soluble in alcohol and most flavor oils at the rate of 3 to 8 %.

Volatile with steam, sublimes before 100° C.

Caramellic-sweet, but rather pungent odor of good tenacity.

First sour, then sweet, caramellic-fruity, bread-like taste, depending upon the concentration used. Sour taste is mostly noticed in very high concentrations of the material.

This material (*iso*-Maltol) which has been identified in baked bread, has not achieved the popularity of Maltol, which is also more stable. Maltol is more versatile and lends enormously sweet fruity notes besides of its caramellic effect.

Not a common commercial product, this item is included for the sake of completing the picture of Maltol isomers.

Prod.: from Lactose via its galactoside.

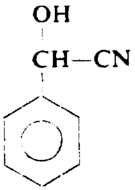
Allo-Maltol is produced from Kojic acid (*5*-Hydroxy-*2*-hydroxymethyl-*gamma*-pyrone) which is obtained by means of biological synthesis.

Kojic acid is also a naturally occurring component of Japanese Sake (ricewine).

69-830; 157-472; 157-480; 158-165;
see also Maltol, previous monograph.

## 1833: dl-MANDELONITRILE

Benzaldehyde cyanohydrin.
*alpha*-Hydroxy-*alpha*-toluic nitrile.



$C_8H_7NO = 133.15$

White prismatic crystals or yellowish oily liquid. Crystals melt at 22° C., one modification melts at minus 10° C. Decomposes under heating. B.P. 170° C. Sp.Gr. 1.12.

Insoluble in water (decomposes), soluble in alcohol and oils.

This material has been used to prepare the so-called "Bitter Almond Water", a mild flavor corrigens employed in pharmacy.

The prescription reads:

| | |
|---|---|
| 11 grams | Mandelo nitrile |
| 500 grams | Alcohol |
| 1489 grams | Water |

to yield 2000 grams of the flavored water. This preparation contains 0.1% hydrocyanic acid. Accordingly, the lethal dose of the Bitter Almond Water is about 20 grams. It has the approximate strength of triturated Bitter Almonds.

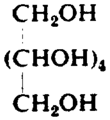
As a food flavoring agent, this preparation is abandoned in most countries, and replaced with dilutions of Benzaldehyde.

Prod.: from Benzaldehyde with Sodium bisulfite and Sodium cyanide.

26-594; 68-901; 68-903; 100-633; 160-1086; B-X-206;

## 1834: MANNITOL

Manna sugar.
*d*-Mannitol (is the most common in Nature).
Mannite.
*1,2,3,4,5,6*-Hexanehexol.



$$\begin{array}{l} CH_2OH \\ | \\ (CHOH)_4 \\ | \\ CH_2OH \end{array}$$

$C_6H_{14}O_6 = 182.18$

White crystals. M.P. 168° C.
16% soluble in water, 1% soluble in alcohol. Insoluble in most oils.

Practically odorless.

Sweet, bland or mild taste, about 0.5 to 0.6 times the sweetness of sugar, when compared in 5 to 10% strength in aqueous solution.

This carbohydrate is used as a food additive, rather than as a flavor item, partly because of its insolubility in flavor materials, partly because of its mild effect as a flavor chemical.

It finds limited use as a low-sweetening and filling additive in powder formed food products, etc. It is not as hygroscopic as Glucose.

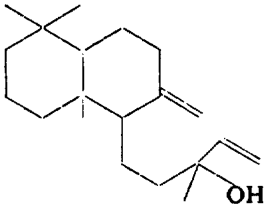
Prod.:

1) as a natural isolate from Manna by boiling with alcohol.
2) synthetic – by electrolytic reduction of Glucose.

1-320; 30-142; 66-1227; 100-637; 160-1086; B-I-534;

## 1835: MANOOL

A bicyclic terpenealcohol.



$C_{20}H_{34}O = 290.49$

The commercial product is a whitish or very pale yellowish crystalline mass or waxy mass. M.P. 53° C. B.P. higher than 320° C. Sp.Gr. 0.97.

Practically insoluble in water, soluble in alcohol, miscible with most oils.

Very delicate, woody, dry-sweet, and extremely tenacious odor with a distinct and typical Ambregris-like undertone.

This alcohol, although known for many decades, has aroused increasing interest during the past 10 or 15 years, particularly since its structure became known and it was evident that it has a definite structural similarity to odorous components of natural Ambergris. It is also very closely related to the chief component of Clary Sage absolute, Sclareol (see that monograph).

Manool, as such, finds only limited use in perfumery. Most of the annual world production – which could be augmented into tens of tons – goes into the production of Ambregris chemical specialties. See also monographs:

Fixateur 404 – and: Ethyl dodecahydro trimethyl naphthofuran.

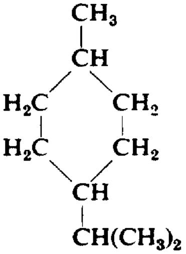
The Dihydro-manool and Tetrahydro-manool are also solid materials but have much weaker odor.

Prod.: by extraction of comminuted wood of Dacrydium biforme, a tree indigenous to New Zealand, with alcohol or Acetone. The extract is neutralized with alkali, and the crude Manool may be recrystallized.

67-715; [illegible] 365; 156-367;
samples and information also from: Timber Processing Co. Auckland, New Zealand.

## 1836: para-MENTHANE

*1*-Methyl-*4*-*iso*-propylcyclohexane.
Hexahydro-*para*-cymene.
Menthonaphthene.
Terpane.



$C_{10}H_{20} = 140.72$

Colorless moblile liquid. Sp.Gr. 0.80.
B.P. 168° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in diluted alcohol.

Somewhat harsh, gassy and sweet odor, reminiscent of Fennel, and of poor tenacity.

This hydrocarbon finds a little use in perfumery, usually in technical (impure) grade, partly for masking or industrial perfumery, partly as a minor component in certain artificial essential oils. It does not occur in Nature, and is not a very desirable material as such, but it serves mainly as an intermediate in the manufacture of various perfume and flavor materials.

Prod.:

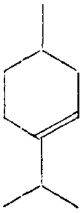
1) by electrolytic reduction of Menthone.
2) by catalytic hydrogenation of *para*-Cymene.

Method No. 2) is the most commonly employed, and the least expensive.

31-7; 31-88; 30-238; 65-19; 67-534; 67-506; 85-81; 87-26; 160-1088;

## 1837: MENTHENE

*para*-Menth-*3*-ene.
*d*-*4*-*iso*-Propyl-*1*-methyl-*3*-cyclohexene.
Menthomenthene.
(Six structurally isomer Menthenes, plus 5 optical isomers).



$C_{10}H_{18} = 138.25$

Colorless mobile liquid. Sp.Gr. 0.81.
B.P. 168° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Typical "hydrocarbon"-odor, similar to that of *para*-Cymene, rather harsh, but in extreme dilution quite refreshing, almost citrusy. Poor tenacity.

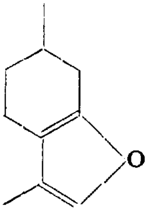
This hydrocarbon, rarely offered commercially, finds a little use in perfumery, mainly in the preparation of artificial essential oils. However, a fairly pure grade of this chemical is comparatively expensive and the odor value of the material does not compensate for the market price of it. Unless it is made available at a price near that of the Citrus terpenes, there is little chance that this terpene will become a standard perfume raw material.

Prod.: by dehydration of Menthol. It has also been prepared by catalytic hydrogenation of Limonene (Platinum catalyst) or Dipentene (Nickel).

31-7; 67-535; 85-81; 160-1088;

## 1838: MENTHOFURAN

*3*,*6*-Dimethyl-*4*,*5*,*6*,*7*-tetrahydrocoumarone.



$C_{10}H_{14}O = 150.22$

Colorless mobile liquid. Easily oxidized in air and daylight, and it will become darker of color, more viscous. Sp.Gr. 0.96.
B.P. 196° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet, haylike-minty odor, sometimes referred to as "Lactone"-odor. Moderate to poor tenacity. The initial impression is that of a very pungent and sharp odor.

The taste – in dilutions lower than 10 ppm – is slightly bitter, almost tarry and not very pleasant.

This material – still important as an analytical key to the identification of Mentha piperita oil – has found a little use in flavor compositions, mainly as a minor component in artificial "Peppermint" oils, based upon Mentha arvensis oils.

Unfortunately, the reaction upon which the analytical identification of Peppermint oil is based, may also be obtained with Pennyroyal oil, the chief component of which is an imtermediate in the synthetic preparation of Menthofuran.

Menthofuran is generally considered an undesirable component of Peppermint oil, and oils of "low Menthofuran content" are often preferred for flavor. The Menthofuran content varies with the maturity of the plant. A considerable proportion of the Menthofuran in a Peppermint oil can be removed by vacuumdistillation. The Menthofuran is concentrated in the foreruns of the distillation.

Prod.:

1) by isolation from "high-Menthofuran"-bearing Mentha piperita oils.
2) from Pulegone by treatment with Sulfuric acid, Sulfuric anhydride and Acetic anhydride, followed by pyrolysis.

The Pulegone may be isolated from Moroccan Pennyroyal oil.

86-85; 89-237; 90-758; 104-514;

## **1839:** dextro-**MENTHOL**

*d*-Menthol.
*d*-Neomenthol (included in this monograph).
Structure: see Menthol.
Out of 12 Menthol isomers, only a few have commercial interest.

$C_{10}H_{20}O = 157.27$

Colorless liquid. B.P. 212° C. Sp.Gr. 0.90.

Almost insoluble in water, soluble in alcohol and oils.

Pungent, woody-minty, slightly camphoraceous odor.

Somewhat bitter, sharp and rather unpleasant taste.

Mixtures of *d*-Menthol and *d*-Neomenthol occur as commercial products obtained from the reduction of *d*-Menthone and *l*-Menthone. The commercial product known as "racemic Menthol" may also contain these isomers in various proportions.

Low-cost mixtures of these materials are used in perfume compositions to give power and "lift" to fragrances, mainly soap perfumes or detergent fragrances, etc.

Due to the unpleasant flavor and lack of cooling effect, *dextro*-Menthol and mixtures containing that Menthol are of little or no interest to the flavorist.

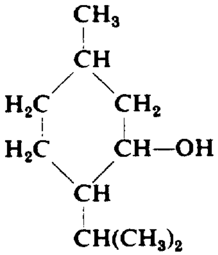
Prod.: by Meerwein-Ponndorf-Verley reduction of *l*-Menthone, resulting in approximately two-thirds *d*-Neomenthol plus one-third *l*-Menthol.

It can also be produced by reduction of *d*-Menthone.

4-85; 26-594; 31-88; 65-226; 86-86; 88-27; 88-37; B-VI-28;

## **1840:** laevo-**MENTHOL**

*l-3-para*-Menthanol.
*5*-Methyl-*2*-*iso*-propyl cyclohexanol.
*5*-Methyl-*2*-*iso*-propyl hexahydrophenol.
"Peppermint camphor".



$C_{10}H_{20}O = 156.27$

Colorless crystals. M.P. 43° C. B.P.216° C. Sp.Gr. 0.90 (liquid).

0.05% soluble in water. Soluble in alcohol and Propylene glycol. Miscible with oils, fairly soluble in Mineral oil and Glycerin.

Refreshing, light, diffusive odor with a sweet pungency. Characteristic resemblance to main odor of Peppermint, and a cooling effect upon the mucous membranes. However, the cooling effect is not perceptible at the same low level at which the material is olfactorily perceptible.

Cooling mouthfeel, refreshing, sweet taste reminiscent of part of the Peppermint picture. At very low concentrations, there is no cooling effect, but still a perceptible flavor.

*l*-Menthol, synthetic or natural, is widely used in perfumes and flavors. Its main use is in flavors as a fortifier for Peppermint flavors, or as a flavor ingredient with a cooling effect and little or no typical bouquet notes of Peppermint.

Smaller amounts are used in perfumes to give refreshing lift and power, mainly to Rose, Geranium, Lavender, Fougere and similar types. Concentrations from 0.5 to 2.5% are usually required to achieve such effects in a perfume.

Separately from the addition of a perfume to certain cosmetic products, Menthol may be added to introduce a cooling effect in shave creams, after-shave lotions, etc. The amount of Menthol may be higher than the total amount of perfume in such cases.

Apart from its conventional role in Peppermint, Spearmint and other Mint flavors, Menthol is used in traces in imitation Butter, Caramel, fruit complexes, etc. and very often along with Anise or Anethole in Licorice flavorings.

The concentration in the finished product will normally be 35 to 400 ppm, but it can reach 1000 to 1200 in chewing gum or dentifrice (the latter being a non-edible product, therefore rarely included in such statistics).

G.R.A.S. F.E.M.A. No.2665.

Prod.:

1) Natural: by freezing from Mentha viridis of Mentha arvensis oils. The Menthone-rich liquid phase may yield further quantities of Menthol (*laevo-* and racemic) by catalytic reduction, normally with Sodium.
2) from Thymol or Piperitone by hydrogenation, or from *laevo-iso-*Pulegol or Citronellal via Pulegol to Menthol.

Numerous other methods and variations of above methods are used in the manufacture of synthetic Menthol. It is estimated that more than 50% of the world production of *l*-Menthol is obtained as "Natural Menthol". Figures referring to production of Natural Menthol in China (mainland) are unavailable or incomplete, but estimates put the annual (China Mainland) production higher than 1000 tons, perhaps higher than 2000 tons. Brazilian production has fluctuated between 700 tons and 2500 tons over the past two decades.

26-594; 4-85; 30-150; 31-21; 30-238; 65-216; 77-152; 85-81; 86-86; 88-28; 88-38; 100-644; 104-413; 106-231; 160-1090;

## 1841: dl-MENTHOL

*racemic-*Menthol.
Hexahydrothymol.
*dl-*Neomenthol (often included in commercial product).
Structure: see Menthol (*laevo-*).

$C_{10}H_{20}O = 156.27$

Colorless crystalline mass. M.P. 51° C. (many commercial products have lower melting point). Sp.Gr. 0.89 (liquid). B.P. 211° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils. Slightly soluble in mineral oil and Glycerin.

Odor very similar to that of Menthol, but somewhat more woody, not quite as sweet, and the cooling sensation is not perceptible at the same low concentration as it is in *laevo-*Menthol.

The taste follows the above odor pattern in that it is less sweet than *laevo-*Menthol, but not bitter as Menthone. It is less cooling on the mucous membranes (and the skin) than *l*-Menthol.

It seems to be the general opinion that *dl*-Menthol comes second to *laevo*-Menthol with respect to acceptability as a "mint"-material. There are flavorists who prefer some of the Neo-isomers, but in view of the difficulty in manufacturing these in reasonable state of purity at a price lower than that of *laevo*-Menthol, preference comes in for *dl*-Menthol.

It is used extensively in perfumes as a cheaper material where *laevo*-Menthol could be used, but the saving is actually negligible since the price difference is rather small and the useful concentration of Menthol in a perfume is low.

In flavors, or in cosmetic preparations, where Menthol is sometimes used in quantities that amount to tens of tons annually for the manufacturer, the savings in using *racemic*-Menthol as partial replacement for *laevo*-Menthol is more obvious. However, a careful evaluation will normally reveal that there is a distinct limit to the extent of such substitution. Particularly in toothpaste flavors, Peppermint candies, chewing gum, etc.

See also comments under: *laevo*-Menthol.

Prod.: (many methods) e. g. by reduction of *dl*-Menthone with Sodium in Ethylether, or by Meerwein-Ponndorf-Verley reduction.

4-85; 86-86; 88-27; 88-38; 106-231;

## 1842: iso-MENTHOL

(Several isomers are known, but few are offered commercially in a pure state).

*dextro-iso*-Menthol: M.P. 82° C.
B.P. 219° C. Sp.Gr. 0.90.
*laevo-iso*-Menthol: liquid. B.P. 206° C.

Various mixtures of *iso*-Menthols are manufactured by Meerwein-Ponndorf-Verley reduction of *iso*-Menthone, obtained from Piperitone by hydrogenation.

These products find limited use in perfume compositions, mainly as low-cost replacements for *laevo*-Menthol in fragrances where a fresh non-citrusy and non-woody "lift" may be desirable. It is mainly applied to soap perfumes and detergent fragrances.

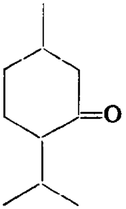
See also notes under: *laevo*-Menthol.

4-85; 86-86; 88-27; 88-38;

## 1843: MENTHONE

*para*-Menthan-*3*-one.
*4-iso*-Propyl-*1*-methylcyclohexan-*3*-one.

*dextro*-Menthone and *laevo*-Menthone are both commercially available, but the latter is the most interesting and attractive to the creative perfumer.



$C_{10}H_{18}O = 154.25$

Colorless oily liquid. Sp.Gr. 0.90.
B.P. 204° C. (*dextro*-) or 207° C. (*laevo*-).

Slightly soluble in water, soluble in alcohol and oils.

Minty-refreshing and diffusive odor of moderate tenacity and slightly woody-dry undertones.

Refreshingly cool, but also unpleasantly bitter taste in dilutions of 10 to 50 ppm.

This ketone finds good use – although always in small proportions – in perfume compositions, Geranium bases, Lavender compositions, Rose or Spice fragrances, etc. It blends well with the Fougère theme and traces can be used to give the lift that is missing in Citronellol for delicate floral compositions, etc.

Menthone is also used in flavor compositions, not only in Mint complexes, but in traces in fruit blends, particularly in imitation Raspberry, where it gives good lift and freshness in the otherwise oversweet composition.

The concentration is normally about 5 to 50 ppm in the finished product.

Prod.:

1) by isolation from Peppermint oil
2) from *para*-Menth-*3*-ene.

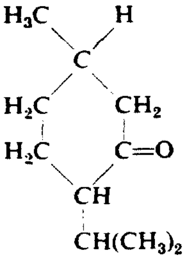
G.R.A.S. F.E.M.A. No.2667.

4-86; 31-88; 85-84; 89-196; 103-232; 106-234; 160-1090; 36-366;

## 1844: iso-**MENTHONE**

*para*-Menthan-*3*-one.

Most commercial products are: *dl-cis-para*-Menthan-*3*-one, and a content of 8 to 12% Menthone is a normal occurrence.



$C_{10}H_{18}O = 154.25$

Colorless, slightly oily liquid. Sp.Gr. 0.90. B.P. 208° C. (up to 212° C. for certain grades).

Almost insoluble in water, soluble in alcohol, Propylene glycol, mineral oil and perfume and flavor materials. Very poorly soluble in Glycerin.

Powerful, refreshing and clean-minty odor of moderate tenacity. Somewhat cooling mouthfeel and refreshing, minty, but distinctly bitter taste.

This ketone was once a comparatively rare and expensive raw material. A temporary situation of high market price and poor supply of Geranium oils encouraged research work on the commercial production of this material to make it available at an attractive price. The price of Geranium oil has since leveled off to a price where many users have abandoned the idea of making an "artificial" or "reconstructed" oil. However, there are other uses for *iso*-Menthone. It gives very interesting effects in Rose, Carnation, Muguet, Fougères, Lavender-complexes, etc. The use-concentration will normally be about 0.5 to 2%, but may be somewhat higher in Rose and Lavender. With the spicy notes in certain types of Men's fragrances, it can eliminate the unpleasant sweetness brought about by the conventional Spice and Fougère fixatives.

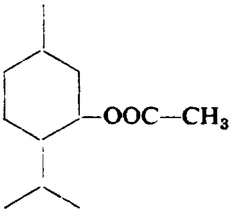
Prod.:

1) by isolation from Moroccan Pennyroyal oil (*dextro*-Menthone).
2) by isolation from Congo Geranium oil (*laevo*-Menthone).
3) synthetic from *3*-Methylcyclohexanone via its Glyoxylester and the corresponding Ketal to *iso*-Pulegone. This ketone is then treated with alcoholic Sodiumethylate to yield *dl*-Pulegone, which is hydrogenated to *iso*-Menthone (*dl-iso*-Menthone).

4-72; 65-390; 67-515; 67-523; 89-204; 89-235; (See also The Trubek Chemical Co. data sheet Febr. 1963, now the U.O.P. Chemical Co., Div. of Universal oil Products, Inc.).

## 1845: laevo-MENTHYL ACETATE

*l-para*-Menth-*3*-yl acetate.



$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Sp.Gr. 0.92. B.P. 227° C.

Very slightly soluble in water, miscible with alcohol and oils. Slightly soluble in Propylene glycol, poorly soluble in Glycerin.

Mild and sweet, slightly fruity-herbaceous, minty odor. Quite refreshing and delicately floral.

Cool mouthfeel, sweet taste with only a trace of mintiness.

Overall much milder than *laevo*-Menthol, more delicate and floral.

This ester finds some use in perfumery, partly as a component of various artificial essential oils, partly as a minor component of floral fragrances, mainly Rose, Muguet, etc. and Oriental or Citrus types. It performs well in soap, giving an interesting lift without the normally unwanted mintiness.

It finds more use in flavor compositions, in various fruit complexes, Mint and Spice combinations, artificial Peppermint and Spearmint, in Cherry (European type, or the American "Bing" Cherry type), etc. Concentrations are usually 5 to 25 ppm in the finished product.

A particularly interesting and specific application of this ester is in certain types of chocolate or fondant-"filling" flavors, where a "cool" feeling along with the Chocolate-Nut-Almond-paste is desirable. Smaller amounts of *laevo*-Menthyl acetate in the flavor gives it the cool mouthfeel, yet adds no trace of minty flavor to the composition (in which Mint usually does not belong). Many types of "Ice" or "cool" chocolate, truffle, etc. are prepared with this material in the flavor composition.

Prod.: by direct esterification of *laevo*-Menthol with Acetic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2668.

4-86; 30-412; 86-87; 90-287; 100-645; 103-98;

## 1846: dl-MENTHYL ACETATE

*racemic*-Menthyl acetate.
Structure: see *laevo*-Menthol.

$C_{12}H_{22}O_2 = 198.31$

Colorless liquid. Sp.Gr. 0.93.

Slightly soluble in water and Glycerin. Soluble in alcohol, Propylene glycol and oils.

Mildly minty and somewhat woody-herbaceous odor. Less floral-fruity and less delicate than the *laevo*-Menthyl acetate.

The taste is also less cooling, but not bitter. More herbaceous with a trace of heavy-fruity, Plum-like undertones.

This ester is used in the same way as the *laevo*-Menthylacetate, but it is inferior when it comes to cooling mouthfeel and delicately floral-fresh notes (e. g. for Muguet, etc.).

It finds some use in soap perfumes, where price is a heavy factor, but it is not frequently used in flavor compositions.

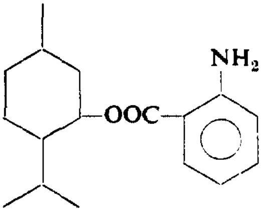
For general perfumery work, however, it gives quite satisfactory results, and it finds many new applications in variations of Men's fragrances, Fougères, Chypres, etc.

Prod.: by direct esterification of *racemic*-Menthol with Acetic acid under azeotropic conditions.

33-504; 106-236;

## 1847: MENTHYL ANTHRANILATE

*para*-Menth-*3*-yl anthranilate.



$C_{17}H_{25}NO_2$ = 275.40

Colorless or pale straw-colored crystals.
M.P. 63° C. The liquid material may remain supercooled and liquid at room temperature for a considerable length of time. Sp.Gr. 1.04. B.P. higher than 300° C.

Insoluble in water, soluble in alcohol and oils. Almost insoluble in Propylene glycol.

Mild, sweet-floral odor of great tenacity. Considerable variations in the odor are noticed when studying samples from different manufacturers.

This ester finds a little use in perfumery as a modifier in sweet floral bases, Neroli, Freesia, etc. Its effect varies from floral to minty or Grape-like.

Menthyl anthranilate is also used as a sunscreening agent in skin lotions.

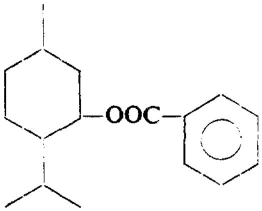
The author has no record of its use in flavor compositions.

Prod.: from Isatoic anhydride (or Isatoic acid) and Menthol.

4-86; 34-1011; 86-87;

## 1848: MENTHYL BENZOATE

*para*-Menth-*3*-yl benzoate.



$C_{17}H_{24}O_2$ = 260.38

Colorless viscous oil.

Insoluble in water, soluble in alcohol and oils.

Very weak, slightly herbaceous-sweet odor of considerable tenacity.

This ester has found some use as a sunscreening agent. To the author's knowledge, it is not used as a fragrance material in perfumes (or flavors). However, since it does have a faint odor, it is briefly mentioned in this work.

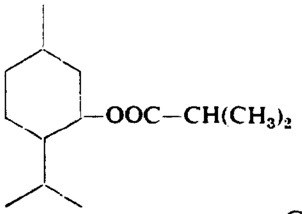
Being a non-phenolic chemical, it has a slight advantage over Menthyl salicylate, but it seems that the latter is still preferred for its sunscreening effect.

Prod.: by azeotropic esterification of Menthol with Benzoic acid.

4-86;

## 1849: MENTHYL-iso-BUTYRATE

*para*-Menth-*3*-yl-*iso*-butyrate.



$C_{14}H_{26}O_2$ = 226.36

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils. Slightly soluble in Propylene glycol, almost insoluble in Glycerin.

This ester is very rarely offered commercially, and does not seem to have achieved much popularity among perfumers or flavorists.

It has a mild, sweet-herbaceous odor reminiscent of Clary Sage with a rosy undertone and good tenacity.

The taste is sweet, deep-fruity, slightly Plum-like.

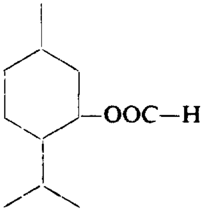
The author is not aware of any significant use of this ester in perfumes and flavors.

Prod.: by direct esterification of Menthol with *iso*-Butyric acid preferably under azeotropic conditions.

28-544;

## 1850: MENTHYL FORMATE

*para*-Menth-*3*-yl formate.



$C_{11}H_{20}O_2 = 184.28$

Colorless liquid. Solidifies in the cold, melts at 9° C. B.P. 208° C.

Very slightly soluble in water, soluble in alcohol and oils.

Herbaceous-refreshing and slightly minty odor with an earthy-green undertone. Moderate tenacity. Some observers find a Narcissus-like floralness. Sweet-herbaceous and slightly minty taste with a floral undertone.

This ester is rarely offered commercially, and apparently of very little interest to the perfumer or flavorist.

It could possibly find use as a minor component in certain variations of Rose, Lily, Muguet, Carnation, etc. where a fresh note in the floral topnote is often desirable.

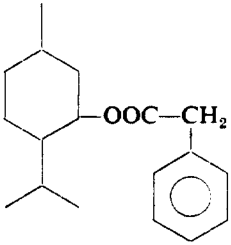
The author is not aware of any significant use of Menthylformate in flavors.

Prod.: by direct formylation of Menthol.

4-86;

## 1851: laevo-MENTHYL PHENYLACETATE

*para*-Menth-*3*-yl phenylacetate.



$C_{18}H_{26}O_2 = 274.41$

Colorless, slightly viscous liquid. B.P. 298° C. Sp.Gr. 0.99.

Insoluble in water, soluble in alcohol, miscible with most oils. Poorly soluble in Propylene glycol, almost insoluble in Glycerin.

Possibly a minor component of Peppermint oil, this ester has found occasional use in perfume compositions where its mild-floral and extremely sweet and tenacious notes can be useful, e. g. in Frangipanni, Honeysuckle, Oriental fragrance types, etc.

It gives interesting and useful effects in Cassie bases, and blends very well with the Ionones, "rose alcohols" Patchouli oil, Styrax, etc.

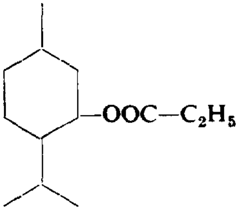
The ester remains, however, a rare and infrequently used material, and its use in flavors is equally unconventional.

Prod.: from Menthol and Phenylacetic acid by azeotropic esterification.

86-87;

## 1852: MENTHYL PROPIONATE

*para*-Menth-*3*-yl propionate.



$C_{13}H_{24}O_2 = 212.34$

Colorless oily liquid. B.P. 222° C.

Almost insoluble in water, soluble in alcohol and oils.

Mild and sweet herbaceous-floral odor with resemblance to Rose and Peony and with a trace of minty undertones. Good tenacity.

Sweet, deep-fruity and somewhat herbaceous-green or balsamic taste with some resemblance to Plum and Melon. There is a cooling mouthfeel at higher levels of concentration, depending upon the type of Menthol used in the esterification.

This ester is only occasionally used in perfume formulations, mostly as a variation and modifier of Menthylacetate in mild floral fragrances, Oriental types, herbaceous Fougères, etc.

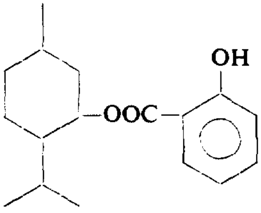
It finds also a little use in flavor compositions as a modifier for the Acetate in mint flavors, in "cool" chocolate compositions without minty flavor, and in certain imitation fruit flavors, e. g. Plum, Prune, Cherry, Melon, etc.

Prod.: by direct esterification of Menthol with Propionic acid or Propionic anhydride.

4-86;

## 1853: MENTHYL SALICYLATE

*para*-Menth-*3*-yl salicylate.
"Antisolaire".



$C_{17}H_{24}O_3 = 276.38$

Colorless oily liquid, or pale straw-colored oily, slightly viscous liquid.
Sp.Gr. 1.05. B.P. approximately 322° C.

Almost odorless when pure. Slightly bitter-astringent taste.

This ester has found some use as a sunscreening agent, but has largely been substituted by Homomenthyl salicylate (see that monograph).

It carries the usual characteristics of a phenol, which are not exactly welcome by the perfumer. It comes in a variety of qualities, some brands having a perceptible odor of Phenol.

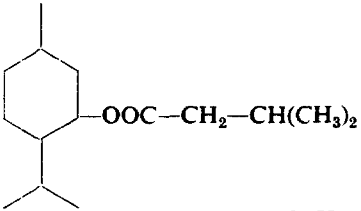
The author is of the opinion that the subject material will become obsolete as a fragrance material and that it does not rank among the most effective sunscreening agents.

Prod.: by azeotropic esterification of Menthol with Salicylic acid, using a Benzene- or Toluene sulfonic acid catalyst.

4-86; 34-788; 86-87; 100-645;

## 1854: MENTHYL-iso-VALERATE

*para*-Menth-*3*-yl-*iso*-valerate.
"Validol" (a pharmaceutical preparation for seasickness).
Commercial products are occasionally called Menthyl valerate.



$C_{15}H_{28}O_2 = 240.39$

Colorless oily liquid. Sp.Gr. 0.91.
B.P. 241° C.

Insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, somewhat balsamic-minty and root-like odor of good tenacity.

Bitter-woody, herbaceous-earthy taste.

This ester finds very little, if any, use in perfumery. It is used sparingly in various flavors, e. g. imitation Plum and other fruits, in mint complexes and in certain types of Liqueur flavors, e. g. the D.O.M. type (which can hardly be approached without the liberal use of natural tinctures).

The concentration is normally about 5 to 20 ppm in the finished product.

Prod.:

1) from *laevo*-Menthol plus *iso*-Valeryl chloride.
2) from *laevo*-Menthol and *iso*-Valeric acid under azeotropic conditions.

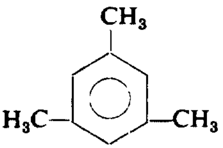
The second method may produce materials of better than 92% ester content, while the first method often leads to a 70-72% ester material. Many commercial products show ester contents as low as 70% and as the balance is mainly Menthol, it is obvious that the odor of such material is substantially different from that of the high-ester product.

G.R.A.S. F.E.M.A. No.2669.

4-86; 7-268; 7-329; 86-87; 90-297; 100-645;

## 1855: MESITYLENE

*symmetric*-Trimethyl benzene.
*1,3,5*-Trimethylbenzene.



$C_9H_{12} = 120.20$

Colorless liquid. Sp.Gr. 0.86. B.P. 165° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Aromatic-herbaceous, ethereal odor, comparatively diffusive, reminiscent of Thyme, overall pleasant, not as gassy as Cymene.

This hydrocarbon has occasionally been used as a masking agent in industrial fragrances, e.g. solvent masks, etc. Its use in perfumery is very limited, partly due to its odor type, partly because the material is rather volatile and difficult to tame by fixation.

Prod.:

1) from Acetone by dehydration with sulfuric acid.
2) also isolated from coal tar naphta.

1-394; 26-708; 31-6; 66-101; 66-108; 100-657; 160-1090; B-V-406;

## 1856: MESITYL OXIDE

*4*-Methyl-*3*-penten-*2*-one.
*iso*-Propylidene acetone.

$CH_3—CO—CH{=}C(CH_3)_2$

$C_6H_{10}O = 98.15$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 130° C.

3% soluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

The commercial grade has an unpleasant

odor, somethimes gassy, green or vegetable-pungent, acrylic.

However, the pure material has a fairly pleasant odor, almost honey-like in dilution – reminiscent of *iso*-Phorol and *iso*-Phorone, and one can observe a breadlike sweetness in this volatile fragrance.

This ketone finds a little use as a masking agent in industrial perfumes. It should be kept in mind that the ketone is unstable under acid conditions (quite frequently prevalent in such end products), and that it will produce Acetone under such circumstances.

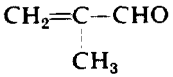
The vapors are moderately hazardous, irritating to the human mucous membranes and skin.

Prod.: from Acetone or Diacetone alcohol by reacting with Iodine or with other dehydrating agents.

1-176; 26-596; 31-84; 66-532; 100-657; 160-1092; B-I-736;

## 1857: METHACROLEIN

Methacrylaldehyde.
*iso*-Crotonaldehyde.
*2*-Methyl propenal.
*alpha*-Methyl acrolein.
"Artemisal".
NOTE: Do not confuse this with:
*meta*-acrolein $(CH_2{=}CH{-}CHO)_3$



$$\underset{\displaystyle CH_3}{CH_2{=}\overset{}{C}}{-}CHO$$

$C_4H_6O = 70.09$

Colorless mobile liquid. Sp.Gr. 0.83.
B.P. 68° C.

6% soluble in water, miscible with alcohol and oils.

Extremely diffusive, "gassy"-sweet odor, in high concentration pungent and irritating, only in extreme dilution fairly pleasant herbaceous-balsamic and remotely Orange-like.

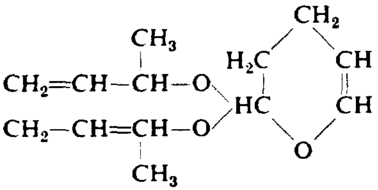
Traces of this aldehyde have been used in the artificial reconstruction of certain essential oils, particularly the herbaceous types.

The material is also used in certain difficult cases of masking of industrial odors.

26-596; 89-37; 160-1092; B-I-731; 35-60;

## 1858: METHALLYL ACETAL DIHYDROPYRAN

*2,3*-Dihydro-*gamma*-pyran di-*alpha-alpha*-methallyl acetal.
*2,3*-Dihydro-*gamma*-pyran di-methyl-vinyl-carbinyl acetal.



$C_{13}H_{21}O_3 = 225.31$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and warm, green-rosy, diffusive odor.

The title material is not offered commercially under its proper chemical name, and the title name – under which it is normally discussed – is not a very accurate chemical name. Acetals of Pyran aldehydes and Acetals, using Hydroxypyrans are often confused and improperly named in perfumery literature.

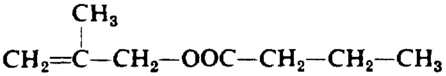
This material finds use in various floral bases and specialties, and it is usually only a minor component of suct products. It contributes power and radiation of the odor, natural warm greenness in the Rose-Geranium character, and it works well with the Rose oxides and related chemicals.

Prod.: from Acrolein by self-condensation by Diels-Alder reaction to *2,3*-Dihydropyran-*2*-aldehyde. The latter is reacted with Methyl vinyl carbinol.

69-840;

## 1859: METHALLYL BUTYRATE

*iso*-Propenyl carbinyl-*n*-butyrate.
*beta*-Methylallyl-*n*-butyrate.
*2*-Methylpropenyl-*n*-butyrate.



$$CH_2{=}\overset{\overset{\displaystyle CH_3}{|}}{C}{-}CH_2{-}OOC{-}CH_2{-}CH_2{-}CH_3$$

$C_8H_{14}O_2 = 142.20$

Colorless mobile liquid. Viscosity increases if the material is exposed to air and daylight, and the odor intensity is simultaneously decreased. B.P. 168° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, penetrating and slightly gassy, overall fruity-ethereal odor of moderate to poor tenacity.

Powerful and rather sharp-acrid taste, except in dilutions below 20 ppm, when the taste is overall sweet, fruity, somewhat sharp but pleasantly reminiscent of Pineapple, Apple, Plum, etc.

This ester, only rarely offered commercially, and not generally approved for food, has found some use in flavor compositions, particularly imitation Pineapple, Apple, "Tropical-fruit" complexes, and in variations of Plum flavor. Concentrations are usually very low, about 0.1 to 0.3 ppm in the finished product.

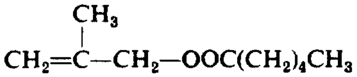
Prod.: by direct esterification of *beta*-Methylallylalcohol with Butyric acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2678.

47-296;

## 1860: METHALLYL CAPROATE

Methylallyl-*n*-hexoate
*iso*-Propenyl carbinyl caproate.
*beta*-Methylallyl caproate.
*2*-Methylpropenyl hexoate.



$$CH_2{=}\overset{\overset{\displaystyle CH_3}{|}}{C}{-}CH_2{-}OOC(CH_2)_4CH_3$$

$C_{10}H_{18}O_2 = 170.25$

Colorless mobile liquid. B.P. 211° C.

Insoluble in water, soluble in alcohol and oils. Viscosity increases if the material is exposed to air and daylight. The odor intensity decreases simultaneously.

Powerful, somewhat pungent-fruity, slightly gassy odor, in dilution reminiscent of Pineapple.

Aqueous dilutions of less than 20 ppm have sweet-fruity, yet slightly sharp or pungent taste, reminiscent of Pineapple or Gooseberry.

This ester has found a little use in flavor compositions, mainly as a modifier in Pineapple imitation flavors or in fruit complexes, occasionally in Rhubarb, Gooseberry or other green-fruity types.

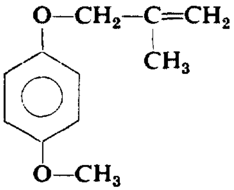
Concentrations are normally mere traces, about 0.1 to 0.5 ppm in the finished product.

Prod.: by direct esterification of *2*-Methylpropenol with Caproic acid under azeotropic conditions.

47-296;

## 1861: METHALLYL-para-METHOXY PHENYLETHER

Hydroquinone methyl methallylether.



$C_{11}H_{14}O_2 = 178.23$

Colorless mobile liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful and sweet; herbaceous-floral odor of Bergamot-type.

Moderate to poor tenacity.

This ether, only recently developed, has been suggested for use in perfume compositions and in artificial Bergamot oils, Bergamot-"extenders" etc.

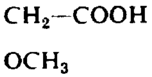
The author has no report of the material being manufactured on a commercial scale, but it may well find use "internally" in the manufacturing houses.

Prod.: from *beta*-Methallylchloride plus Hydroquinone monomethylether in weak aqueous alkali.

(See: American Perfumer & Cosmetics: Vol. 83, April 1968, page 31).

## 1862: METHOXYACETIC ACID

Methyloglycolic acid.
Methoxyethanoic acid.



$$\begin{array}{l} CH_2\text{—}COOH \\ OCH_3 \end{array}$$

$C_3H_6O_3 = 90.08$

Colorless, slightly viscous, hygroscopic liquid. Sp.Gr. 1.18. B.P. 205° C.

Soluble in water, alcohol and oils.

Peculiar fatty vinegear-like odor, in dilution fairly pleasant.

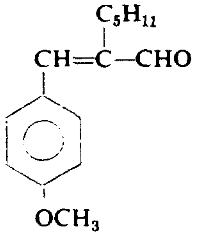
Has been suggested for use in flavor compositions, or as a food additive along with – or replacing – other acidifiers.

Its peculiar aroma seems to limit its application, and it is not commonly used.

Prod.: from Monochloroacetic acid with Sodium methylate.

31-158; 66-788; 160-774;

## 1863: para-METHOXY-alpha-n-AMYLCINNAMIC ALDEHYDE



$C_{15}H_{20}O_2 = 232.33$

Pale yellowish oily liquid. B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Mild, oily-floral and sweet odor of considerable tenacity. There is some resemblance to Acacia or Lilac, but samples from various suppliers show considerable difference in odor type.

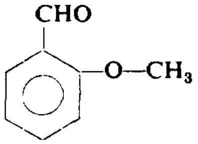
This aldehyde, apparently developed in search of materials more interesting than Amylcinnamic aldehyde, has not achieved much success with the perfumers, and it is only occasionally offered commercially. It seems quite possible that it will become obsolete withing the next decade or two.

Prod.: from *para*-Anisaldehyde plus Heptaldehyde by condensation using a Pyridine type catalyst.

5-144; 86-88;

## 1864: ortho-METHOXYBENZALDEHYDE

Methyl salicylaldehyde.
*iso*-Anisaldehyde.
*ortho*-Anisaldehyde.
Salicylaldehyde methylether.



$C_8H_8O_2 = 136.15$

Colorless or crême-colored crystals or translucent crystalline mass. M.P. 38° C.
Sp.Gr. 1.13 (liquid). B.P. 244° C.

Insoluble in water, slightly soluble in alcohol, miscible with oils.

Faint, sweet-balsamic and floral odor of good tenacity. It appears more "cinnamic" than Anisaldehyde (*para-*) and not as harsh-Hawthorne-like.

This aldehyde, much less known than the *para-*Anisaldehyde ("Aubepine"), finds only a little use in perfumery as a modifier for its *para-*isomer, or in general as a spicy floralizer/fixative.

It blends well with the Cinnamic family, with the Eugenols and with Oriental floral-woody notes, Labdanum, etc.

The aldehyde is used in various flavor compositions, mainly Cassia or other spice blends.

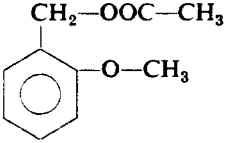
The concentration used is about 20 to 30 ppm in the finished product. It suffers from the same drawback as its isomer in that it cannot be used in higher concentration since its flavor easily turns bitter-"perfumey" when the concentration is raised above 30-50 ppm.

Prod.: by Methylation of Salicylaldehyde with Dimethyl sulfate in weak aqueous alkaline solution.

4-12; 26-414; 68-743; 90-497; 160-828;
B-VIII 43;

## 1865: ortho-METHOXY BENZYLACETATE

"*iso-*Anisylacetate".
*2-*Methylsaligeninacetate.



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid. B.P. 259° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and powerful Rose-like odor of good tenacity. The type is mainly green-balsamic with some resemblance to Hydratropyl alcohol, yet more rosy and powerful.

This ester has been suggested for use in Rose bases for general use in perfume creation. It lends power and sweetness of a more pleasant character than the Phenylacetic acid members do, and it presents an interesting and novel note for experimental Rose bases.

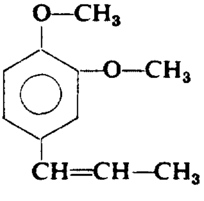
It gives good effects in Cassie bases, and it can be used quite widely in floral and powdery perfume types.

Prod.: by Methylation of Salicylalcohol, followed by esterification with acetic acid under azeotropic conditions.

See also: Ethyl-*ortho-*methoxybenzylether.
Ethyl phenylethyl ether.
Methyl phenylethyl ether.

## 1866: METHOXY-iso-CHAVIBETOL

*1-*Methoxy-*5-*propenylguaiacol.
*iso-*Chavibetol methylether.
*para-*Propenyl catechol dimethylether.



$C_{11}H_{14}O_2 = 178.23$

White crystals. Very slightly soluble in cold water, somewhat better in hot water. Soluble in alcohol and oils, fairly soluble in Propylene glycol.

Sweet Vanilla-like odor with variable amounts of phenolic-medicinal notes, most conceivably appearing in impure materials. Excellent tenacity, and power, particularly when used in combination with related sweeteners.

In dilutions below 10 ppm the taste is fairly sweet, pleasant and Vanilla-like, but at higher concentrations there is an increasing note of tarry or medicinal character. In this respect, the material resembles Propenyl guaethol (Vanitrope).

This phenolether has been suggested for use in perfume compositions, and it is quite useful in the hands of an experienced creative perfumer. It can add missing notes to an artificial Oakmoss composition, and sweetness to floral or Oriental bases, It performs very well with Coumarin, Ethylvanillin, Ionones, Labdanum and artificial Musks, etc.

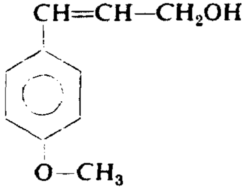
In flavors, it could be used as supporting note in imitation Vanilla or as a modifier along with Ethylvanillin in many caramel, cream, toffee and similar flavor types. Its concentration should be kept at about 1 to 5 ppm in the finished product. There is no published indication that this chemical is officially recognized as safe in the U.S.A. Federal Register, but it is most conceivable that the material is used in number of countries in food flavors.

Prod.: by isomerization of Chavibetol, followed by Methylation with Dimethylsulfate.

(See: Berichte der Deutschen Chemischen Gesellschaft 1941, 74, 832).
(See also: Methyl ethyl-*iso*-eugenol).

## 1867: para-METHOXY CINNAMIC ALCOHOL

*para*-Cumaric alcohol methylether.



$C_{10}H_{12}O_2 = 164.21$

Colorless or white crystals. M.P. 80° C.

Mild, pleasant, floral odor of excellent tenacity. The sweetness and floralness is rather nondescript and it has been described with floral names from Rose to Hyacinth, from Tuberose to Lilac and Acacia.

The major asset of this alcohol is its versatility, making it an excellent background base for floral or Oriental fragrances, Chypres and Fougères, etc. It seems to adjust obediently to the effect of almost all the more volatile components which enter the composition, and only act as a mild blender, fixative and "rounding" agent.

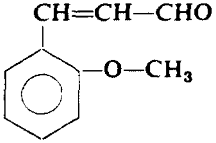
However, the alcohol is not often offered commercially, and it is missing on the shelves of most perfume laboratories. It has strong competition from the low cost alcohols such as Cinnamic alcohol, Hydratropic alcohol, etc. and would have to be made available at a similar price level in order to become truly popular.

Prod.:
1) from *para*-Methoxy alanine.
2) from *para*-Methoxy cinnamic aldehyde by reduction.

68-982;

## 1868: ortho-METHOXY CINNAMIC ALDEHYDE

*ortho*-Cumaric aldehyde methylether.



$C_{10}H_{10}O_2 = 162.19$

Pale yellowish crystals. M.P. 46° C.
B.P. 295° C. (decompos.).

Very slightly soluble in water, soluble in alcohol and oils.

Colors the human skin intensely yellow, particularly when applied in alkaline solution.

Sweet and warm, spicy-floral odor of considerable tenacity. Has a peculiar fruity undertone, resembling notes in Tagetes oil.

Sweet-spicy and warm flavor in dilutions below 200 ppm. Somewhat pungent at higher levels. Resembles Cassia, but is sweeter and more fruity.

This aldehyde is rarely used in perfumes, where its tendency to produce color – and intensifying colors – is a drawback known to the perfumer.

It finds some use in flavor compositions, partly as a modifier for Cassia and Cinnamon spice blends, partly as an interesting additive to Apple and Berry flavor imitations.

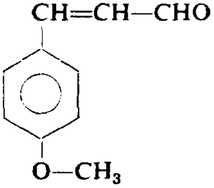
The normal use level is equivalent to about 30 to 200 ppm in the finished product.

Prod.: by condensation of Salicylaldehyde methylether (also known as *ortho*-Anisaldehyde) with Acetaldehyde in alkaline solution.

68-986; 90-532; 95-142; 96-123;

## 1869: para-METHOXY CINNAMIC ALDEHYDE

*para*-Cumaric aldehyde methylether.



$C_{10}H_{10}O_2 = 162.19$

Yellowish crystals. M.P. 58° C. B.P. 277° C.

Almost insoluble in water, soluble in alcohol and oils. Colors the human skin intensely yellow.

Warm and spicy-herbaceous odor. Less fruity and less floral than the odor of the *ortho*-isomer. Good tenacity.

This aldehyde gives interesting effects in herbaceous fragrances, particularly those based upon Lavender and Clary Sage. It supports the fixation of the fragrance, and builds a very natural sweetness with traces of spicy-herbaceous notes, often introduced by the aid of much more expensive oils, such as Estragon and Cinnamon bark oils.

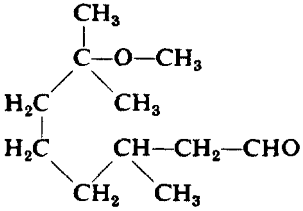
However, the aldehyde suffers from the same drawbacks as many other derivatives of Cinnamic aldehyde – generally believed to be more irritating to the human skin than most other perfume materials, and therefore in obvious danger of being left out of fragrance compositions just for that reason.

Prod.: by condensation of *para*-Anisaldehyde and Acetaldehyde in alkaline solution.

7-268; 31-151; 86-87; 90-533; 95-142;

## 1870: METHOXYCITRONELLAL

*3*,*7*-Dimethyl-*7*-methoxy-*1*-octanal.
Hydroxycitronellal methylether.
"Melonia" (Hoffmann-laRoche).
7-Methoxy-*3*,*7*-dimethyloctan-*1*-al.



$C_{11}H_{22}O_2 = 186.30$

Colorless slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils, fairly soluble in Propylene glycol.

Fresh, somewhat green, floral-sweet Lily-like odor with some resemblance to Hydroxycitronellal and Cyclamal. Good tenacity, but not as much as Hydroxycitronellal.

This aldehyde, surprisingly enough only recently brought into large volume commercial availability, and still priced considerably higher than Hydroxycitronellal, offers many new and interesting uses and novel effects in perfumes.

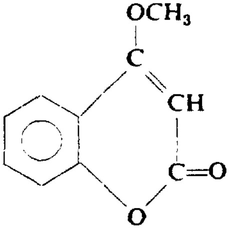
It is used in many types of floral fragrances, in floral bases, particularly recommended for Ylang-Ylang bases, but the author finds it more useful in the fresh-floral types, wholly or partially substituting for Hydroxycitronellal, Cyclamal, Bucinal or similar floral aldehydes. It blends very well with the "rose" alcohols, with the Cinnamic derivatives and with the Eugenols, Benzylacetate and other common ingredients. It needs more fixation than Hydroxycitronellal which in itself is a fixative, but it also offers fresh-green, almost vegetable-green notes, not found in Hydroxycitronellal, and not found so pleasantly effective in Cyclamen aldehyde. Its softness makes it easy to use, hard to overdose, and the same can not be said about Cyclamal.

Prod.: by catalytic Methylation of Hydroxycitronellal.

(Material from H. laRoche Aromatics).

## 1871: 4-METHOXY COUMARIN

An isomer of Methylumbelliferone.



$C_{10}H_8O_3 = 176.17$

Colorless or white crystals. M.P. 98° C.

Practically insoluble in water, very poorly soluble in cold alcohol, slightly soluble in warm alcohol, poorly soluble in most oils.

Faintly herbaceous, sweet and very tenacious odor, but overall disappointingly weak.

This material is briefly mentioned because it has repeatedly been described in literature as a fragrance material.

The author of this work would comment that it has little, if any, mission at all in perfumes or flavors. Its "odor level" is extremely low, its solubility very poor, and its odor type not at all unusual.

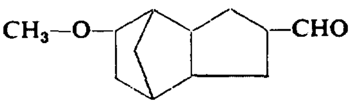
It has not been identified in any natural product, and the author can see no reason to classify this material as a perfume ingredient. This monograph may then serve to cover the alkylethers of Hydroxycoumarins. The *7*-Methoxy coumarin is known as Methylumbelliferone and has had some application as a sunscreening agent, but is, to the author's knowledge, obsolete in that field.

Prod.: from *4*-Hydroxycoumarin with Diazomethane. *4*-Hydroxycoumarin may be obtained from Diphenylmalonate by cyclization with Aluminum chloride. It has also been prepared from Methyl acetylsalicylate by treatment with Sodium in liquid paraffin at 240° C.

68-878;

## 1872: 6-METHOXY DICYCLOPENTADIENE ALDEHYDE

Exo-*3A,4,5,6,7,7A*-hexahydro-*5* (or -*6*-)methoxy-*4,7*-methanoindan-*2*-carboxaldehyde.



$C_{12}H_{18}O_2 = 194.28$

Colorless viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Camphoraceous-woody, slightly green and sweet, Melon-like odor of considerable tenacity.

This aldehyde, much simpler to the organic chemist than it may sound to a perfumer, has been suggested for use in perfume compositions where its powerful and refreshing-green, sweet notes blend well with Sandalwood and Cedarwood, Ionones and Cyclohexylderivatives, Lavandin oil and Geranium compositions, etc.

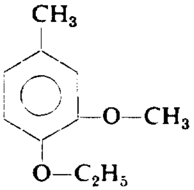
It gives good results in soap and is overall a very stable aldehyde.

The aldehyde is rarely, if ever, offered under its proper chemical name, but it finds use in many perfumes and bases under trade names.

Prod.: from Methoxy dihydro dicyclopentadiene via Oxoreaction.

## 1873: 3-METHOXY-4-ETHOXY METHYL BENZOL

*3*-Methoxy-*4*-ethoxy toluene.
Creosol ethylether. (Note: Cr*eo*sol-).
Homocatechol methylethyl ether.



$C_{10}H_{14}O_2 = 166.22$

White crystals.

Very slightly soluble in water, soluble in alcohol and oils. Slightly soluble in Propylene glycol.

Warm-spicy, Vanilla-like, woody balsamic odor of good tenacity.

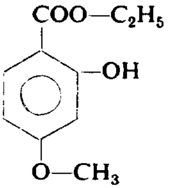
This ether has been suggested for use in perfume compositions and bases. It produces very interesting and lasting notes in Oakmoss compositions, enhances the heavy sweetness of Oriental fragrances, and blends excellently with the Methyl ionones, Patchouli, Sandalwood, Oakmoss, Rose, the Balsams, Castoreum, etc.

In flavor compositions it could find use for imitation Vanilla and as a heavy sweetener for flavors in baked goods, hot-processed candy, etc. on account of its great tenacity.

Prod.: from Catechuic aldehyde (*3,4*-Dimethoxybenzaldehyde) which is reduced to Homocatechol. This is methylated to its Monomethylether, and the Ethylation gives Homoacetechol methyl ethyl ether.

## 1874: para-METHOXY ETHYLSALICYLATE

*ortho*-Hydroxy ethylanisate.
(Occasionally called: "*beta*-Methoxy ethylsalicylate", misleading name).
*2*-Hydroxy-*4*-methoxy ethyl benzoate.



$C_{10}H_{12}O_4 = 196.21$

White colorless crystals.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous odor of Anise-Fennel type, of good tenacity. It seems to have more sweetness and less of a natural herbaceousness than the natural oils which it resembles.

This Phenol-ether-ester has been suggested for use in perfume compositions as a modifier for sweet Salicylates in Lilac or Fougère types, in Chypres or Lavender bouquets.

However, it does not offer any unique or extremely powerful notes not found in the inexpensive natural products, and the chemical will most likely fall into oblivion, except for occasional application in certain rare essential oils or flower absolutes.

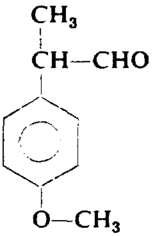
The Methyl-ester is the chief component of the essential oil from the rhizomes of the Primula plant.

Prod.: from Diazoethane plus *beta*-Resorcylic acid.

4-87;

## 1875: para-METHOXY HYDRATROPIC ALDEHYDE

*alpha*-Methyl-*para*-methoxy phenylacetaldehyde.



$C_{10}H_{12}O_2 = 164.21$

Viscous colorless or pale straw-colored liquid. B.P. 239° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful green, sap-like, sweet and somewhat floral odor of moderate tenacity. Some observers describe the odor as "florist-shop"-like, and it is true that the slightly earthy undertones contribute to this more complex, but interesting odor.

This aldehyde is used, although not very widely, in perfume formulations as a modifier for the conventional green and aldehydic-floral notes in Cyclamen aldehyde, Hydratropic aldehyde, etc. It gives interesting effects in Hyacinth, Narcisse, Rose and other florals, as well as in Chypre or Oriental types.

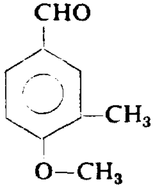
It carries the disadvantage of being rather unstable and it will show a decreasing aldehyde content upon analysis during prolonged storage.

Prod.: from Anethole via Anethole-Iodohydrin.

68-745;

## 1876: 4-METHOXY-3-METHYL BENZALDEHYDE

*meta*-Methyl anisic aldehyde.
*para*-Methoxy-*meta*-tolylaldehyde.



$C_9H_{10}O_2 = 150.18$

White crystals.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-balsamic, earthy-floral odor of considerable tenacity, but relatively weak overall.

The title material is an offspring of the Vanillin research, and it is also related to Anisaldehyde. It has been known for over 70 years, but never seemed to achieve a place in the perfume or flavor laboratory. Its odor is relatively weak, and its taste rather bitter at the level of reasonable perception (about 30 to 50 ppm).

It is safe to state that the title material is practically obsolete in perfume or flavors today.

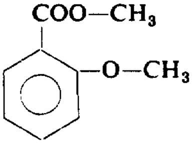
Prod.:

1) from *ortho*-Cresol with Chloroform and Alkali. The resulting *para*-hydroxy-compound is contaminated with *ortho*-hydroxyisomer, and must be purified before Methylation yields the title material.
2) by Diazoreaction upon *4*-Amino-*3*-methylbenzaldehyde, followed by Methylation with Dimethyl sulfate in weak aqueous alkali.

68-744; 72-111;

## 1877: ortho-METHOXY METHYL BENZOATE

Methyl-*ortho*-anisate.
"Dimethyl salicylate" (commercial, confusing name).
Methyl-*ortho*-methoxybenzoate.
Methylsalicylate methylether.



$C_9H_{10}O_3$ = 166.18

Colorless or very pale straw-colored oily liquid. B.P. 246° C. Sp.Gr. 1,16.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-herbaceous-floral, slightly spicy odor with some resemblance to Hyacinth and Cananga. It displays a pleasant, deep-fruity undertone with slight resemblance to Blackcurrant and Grape.

This ester, not frequently used in perfumes, finds occasional application in Hyacinth or Narcisse-bases, various floral-pungent compositions, Oriental fragrances, etc. The *ortho*-Methoxy ethyl benzoate is often preferred (see monograph: Ethyl-*ortho*-methoxybenzoate).

It finds some use in flavor compositions, particularly in imitation Blackcurrant and other berries.

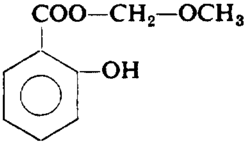
Prod.:
1) by Methylation of Methylsalicylate in alkaline solution with Dimethylsulfate.
2) by esterification of *ortho*-Anisic acid.

G.R.A.S. F.E.M.A. No.2717.

90-565; 7-209; 8-137;

## 1878: METHOXY METHYLSALICYLATE

"Mesotan" (Bayer).
"Ericin".
Salicylic acid, methoxymethylester.
NOTE: Do *not* confuse with: Methyl-*ortho*-methoxybenzoate (see that monograph).



$C_9H_{10}O_4$ = 182.18

Colorless or pale yellowish oily liquid.
Sp.Gr. 1.20. B.P. 246° C.

Slightly soluble in water, soluble in alcohol and oils.

Faint, warm-herbaceous odor with some resemblance to Wintergreen, but sweeter and much milder, somewhat more tenacious.

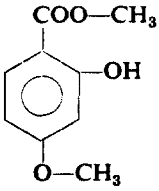
This material is mentioned mainly for the purpose of elucidating the common problem arising from errors in commercial nomenclature particularly in reference to perfume and flavor chemicals.

It is of very little interest to the perfumer or flavorist, but it still finds some use in pharmaceutical preparations.

2-206; 100-658;
see also: 90-566 and 90-567;

## 1879: para-METHOXY METHYLSALICYLATE

*ortho*-Hydroxy methylanisate.
*2*-Hydroxy-*4*-methoxybenzoic acid, methylester.
"Primula Camphor".
Methyl-*2*-oxy-*4*-methoxybenzoate (old name).
NOTE: Do not confuse with: Methyl-*para*-methylsalicylate (see monograph).



$C_9H_{10}O_4$ = 182.18

White or colorless crystals. M.P. 50° C. B.P. 210° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-herbaceous, Wintergreen-Anise-Fennel type odor of moderate tenacity. Overall more pungent and harsh than any of the named naturals, but sweeter than Anisole (Methyl phenylether).

Heavy-pungent fruity taste with a faint resemblance to Blackcurrant.

This Phenol-ether-ester is occasionally used in perfume compositions as a modifier for Methylsalicylate, Anisole, Dihydroanethole etc., mostly in variations of Pine or Fir or Cedarwood fragrances and often for technical or industrial purposes.

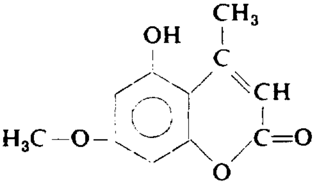
It carries the usual drawbacks of a phenol and its use in fragrances is therefore limited.

Prod.: from Diazomethane plus *beta*-Resorcylic acid.

34-787; 34-789; 90-566; 86-96;
see also monographs on: Methyl methoxybenzoate, *para*-Methyl methylsalicylate, and: Methyl-2-oxy-5-methoxybenzoate.

## 1880: 7-METHOXY-5-OXY-4-METHYLCOUMARIN

7-Methoxy-5-hydroxy-4-methylcoumarin.
(The use of "-oxy-" for the hydroxyl radicle has largely been abandoned in chemical literature, but is still found in perfumery literature).



$C_{11}H_{10}O_4 = 206.20$

White crystals.

Insoluble in water, poorly soluble in alcohol, soluble in most oils, but not freely soluble.

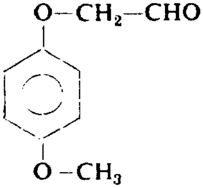
Dry-musty, herbaceous, Leather-like and Tobacco-like odor of considerable tenacity.

The odor is often described as "musky" which is a common description for the odor of materials of very low vapor pressure and with lack of characteristic odor type.

This Coumarin derivative is one of many developed in search of more interesting varieties of the Coumarin-type odor. Its weak fragrance and very poor solubility are drawbacks which could only be compensated for by very low cost or very unusual odor *type*. None of which are pertinent to the title chemical.

The author believes that this chemical, rarely offered commercially, can be considered as practically obsolete and unnecessary for the perfumer and the flavorist.

## 1881: para-METHOXY PHENOXYACETALDEHYDE



$C_9H_{10}O_3 = 166.18$

Colorless or pale yellowish viscous liquid.
Almost insoluble in water, soluble in alcohol and oils.

Sweet-green and somewhat floral odor with good tenacity and rich, sweet, flower-stem-like undertones.

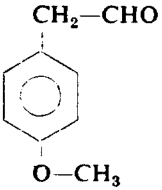
This aldehyde, rarely offered under its proper chemical name, is used in perfume compositions for its powerful green, bark-like and flower-stem-like effect, normally in conjunction with foliage-green or herbaceous-green notes, as a part of a green complex or base. It lends almost honey-like undertones, very useful in variations of Rose, Honeysuckle, Sweet Pea, etc.

Prod.: (several methods) e. g. from *para*-Hydroxy phenoxyacetic acid via its chloride to *para*-phenoxyacetal, which by acid hydrolysis yields subject material.

(See also: 68-428).

## **1882:** para-**METHOXY PHENYLACETALDEHYDE**

Homo anisic aldehyde.
"*para*-Anisyl acetaldehyde" (misleading name).



$C_9H_{10}O_2 = 150.18$

Colorless oily liquid. B.P. 255° C.
Sp.Gr. 1.10.

Slightly soluble in water, soluble in alcohol and oils. Also soluble in Propylene glycol.

Sweet-floral, slightly green odor of good tenacity. It has notes resembling those of Lilac, Heliotrope and Hawthorne at the same time.

This aldehyde is used in perfume compositions as part of the floral theme, mainly in Lilac, Heliotrope, Wallflower, Acacia, New Mown Hay, Hawthorne, and also in Fougères as a sweetener or modifier for Anisaldehyde, etc. It blends excellently with the conventional sweeteners and florals, and produces softer, less harsh notes than Anisaldehyde or the substituted Acetophenones.

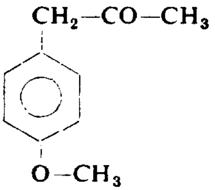
The aldehyde tends to polymerize on storage and should be kept at uniform temperature, preferably in dilution, protected from daylight and air. Polymerization causes increase in viscosity and loss of odor.

Prod.:
1) from *para*-Methoxy allyl benzene with Mercuric oxide plus Iodine.
2) from *para*-Styrylcarbamic ester by hydrolysis with Sulfuric acid.
3) from Anisaldehyde via Darzens' synthesis.
4) It has also been prepared from Estragole.

4-87; 5-125; 36-1027; 61-61; 68-745; 86-88; 86-13; 103-152;

## **1883:** para-**METHOXY PHENYLACETONE**

*1*-(*para*-Methoxyphenyl)-*2*-propanone.
*4*-Methoxy phenylpropanone.
*para*-Anisyl acetone (confusing name, also erroneously for *para*-Methoxy acetophenone).
Anisketone.
Anisic ketone.
Anisyl methyl ketone.
NOTE: see NOTE under: Anisylacetone.



$C_{10}H_{12}O_2 = 164.21$

Colorless or pale straw-colored oily liquid. B.P. 265° C. Sp.Gr. 1.10.

Almost insoluble in water, soluble in alcohol and oils.

Mild, yet somewhat "gassy" Hawthorne-Anise type odor of good tenacity. It has some resemblance to Methylacetophenone, but is not nearly as harsh or pungent.

The subject material is used occasionally in perfumes, but more frequently in flavor compositions.

In fruit and imitation Vanilla, sometimes in Walnut or Cherry flavors, it may be used in traces, equivalent to 0.5 to 5 ppm in the finished product.

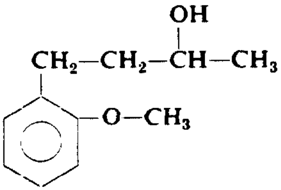
G.R.A.S. F.E.M.A. No.2674.

Prod.:
1) from Anisole and Acetylchloride with Aluminum chloride.
2) from *1*-*para*-Methoxyphenylpropane-*1,2*-diol or its derivatives.

17-44; 31-83; 34-679; 68-752; 74-479; 86-88; 96-157; 103-152; 103-273;

## 1884: ortho-**METHOXY**-4-**PHENYLBUTANOL**-2

*ortho*-Methoxy phenylethyl methylcarbinol.



$C_{11}H_{16}O_2 = 180.25$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and comparatively powerful floral odor with a pronounced green-herbal undertone. The sweetness tends to be almost buttery-creamy, but not more than what is agreeable. The tenacity is good.

This "carbinol" has been suggested for use in perfume compositions mainly of the floral and floral-fruity and floral herbaceous type, in which it introduces novel tonalities and is capable of giving quite interesting effects.

The material is rarely offered under its proper chemical name.

Prod.: by Raney-Nickel type reduction of *ortho*-Methoxy phenylbutanone which is obtained from Acetone and Salicylic aldehyde, followed by hydrogenation.

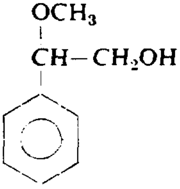
It can also be prepared from *ortho*-Methoxy methyl styryl ketone.

See also: 4-87; 68-988; 86-88;

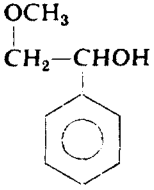
## 1885: 2-**METHOXY**-2-**PHENYLETHYLALCOHOL**

Sometimes called:
Tyrosol methylether (incorrect name)*).
The commercial product, when offered to the perfume industry, has usually consisted of a mixture of two isomers:

1) the title material (main component).
2) *2*-Methoxy-*1*-phenylethanol.



1)



2)

$C_9H_{12}O_2 = 152.20$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and woody-green, moderately floral odor of fair tenacity. The odor is substantially different from that of Phenylethylalcohol, but, in the opinion of most perfumers, not to the advantage of the title material. The odor lacks character and versatility, for which Phenylethylalcohol is popular, in spite of its rather low odor value.

The material has been known for several decades, and the fact that it is still not commonly offered or available should be enough proof that this alcohol is becoming obsolete.

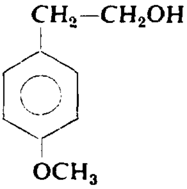
Prod.:

1) from Styrene by catalytic hydrogenation in presence of Methanol and sulfuric acid. This reaction leads to product No. 1) as main component.
2) by hydrogenation of *omega*-Methoxy acetophenone. This reaction leads mainly to product No. 2).

68-878;

see also: 68-736; 163-357;

*) The structure for Tyrosol methylether is:

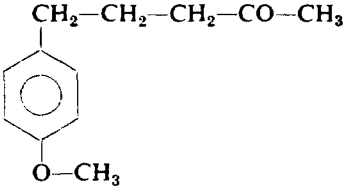


M.P.24° C.

The *ortho*-Methylether is also known.

## **1886:** alpha-(para-**METHOXYPHENYL**)-n-**PROPYL METHYL KETONE**

*para*-Methoxy phenylethylacetone.
*5*-(*4*-Methoxyphenyl)-pentan-*2*-one.
"Homoanisylacetone".
"Dihydroethone".



$C_{12}H_{16}O_2 = 192.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Intensely sweet, creamy-floral odor of good tenacity. The undertones are somewhat herbaceous, but only add to the pleasant, natural overall character. Dilution call out intensely fruity-sweet notes.

This ketone has been suggested for use in perfume compositions, and it finds some use under various trade names.

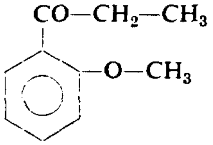
It gives interesting variations from the Heliotropine-theme, and extends the field of application of Heliotropine, Cyclamenaldehyde, Hydroxycitronellal to a great variety of floral nuances and types. It is most likely that it could find use in fruity flavor compositions.

Prod.:

1) from Homoanisaldehyde by condensation with Acetone, followed by hydrogenation.
2) from Anisaldehyde plus Methyl ethyl ketone, followed by hydrogenation (see monograph No. 1907).

## **1887:** ortho-**METHOXY PROPIOPHENONE**

*ortho*-Methoxy phenylethyl ketone.
Ethyl-*ortho*-methoxy phenyl ketone.
*1*-(*ortho*-Methoxyphenyl)-*1*-propanone.
The commercial material contains some *para*-isomer.



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, somewhat pungent, buttery-creamy odor with floral notes upon proper dilution. Moderate to poor tenacity.

This ketone, not a very common perfume chemical, has found a little use as a modifier for the Acetophenone derivatives in floral-woody and floral-herbaceous fragrance types. It gives interesting variations of Mimosa-like effect with Labdanum derivatives or with *iso*-Butyl-cinnamate or similar Labdanum materials.

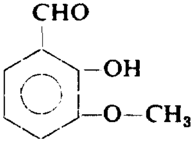
Prod.: by rearrangement of Phenylpropionate with Aluminum chloride in Carbon disulfide solution, followed by Methylation with Dimethyl sulfate in weak aqueous alkaline solution.

Some *para*-isomer is formed during the first step.

3-211; 68-752;

## **1888:** meta-**METHOXY SALICYLIC ALDEHYDE**

*3*-Methoxysalicylaldehyde.
*2*-Hydroxy-*3*-methoxybenzaldehyde.
(An isomer of Vanillin).
»*ortho*-Vanillin«.



$C_8H_8O_3 = 152.15$

Yellowish crystals. M.P. 46° C.

Very slightly soluble in water, soluble in alcohol and oils.

Faint, but very sweet and mildly pungent "medicinal"-Vanilla-like odor with notes recalling Guaiacol, Salicylaldehyde, Coumarin and Vanillin at the same time. Overall not a very attractive combination, but due to the weakness of odor, not really unpleasant.

The title material is briefly mentioned here for various reasons. It has found some use as an antioxidant, mostly in technical products. It occurs as a by-product in the manufacture of Vanillin by the Guiacol-method, and it has once been a problem to remove the title isomer completely from Vanillin made by this method.

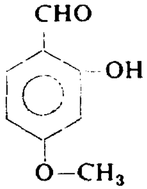
*ortho*-Vanillin is considered more toxic than Vanillin, and it is not used in flavors.

Prod.: as above mentioned.

1-513; 31-151; 68-746; 72-111; 90-514; 140-278; 163-75; 163-243;

## 1889: para-**METHOXY SALICYLIC ALDEHYDE**

*2*-Hydroxy anisaldehyde.
*2*-Hydroxy-*4*-methoxybenzaldehyde.
*4*-Methoxysalicylaldehyde.



$C_8H_8O_3 = 152.15$

White or colorless crystals. M.P. 42° C.

Slightly soluble in water, more in hot water. Soluble in alcohol and oils.

Sweet and very tenacious floral-spicy odor with a somewhat medicinal undertone. Less warm than the *meta*-isomer, and not quite as Vanilla-like.

Sweet, but somewhat pungent and slightly medicinal taste in water.

This material has been suggested for use in perfume compositions as a modifier for Vanillin, Eugenol and their derivatives, particularly in compositions where Oakmoss forms an important part.

However, this material is not regularly available from the usual suppliers of perfumery raw materials, and it can not be produced at a price nearly as low as that of Vanillin.

Most likely, it will remain a research chemical with some academic interest because of its occurrence in certain essential oils.

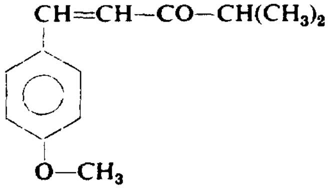
Prod.:

1) by isolation from the essential oils from various East Indian roots.
2) by the Reimer-Tiemann reaction upon Recorcinol monomethylether (yielding the *2,4*- and the *4,2*-isomers).

4-87; 68-748; 90-521;

## 1890: para-**METHOXYSTYRYL**-iso-**PROPYL KETONE**

"Homo ethone".
*1*-(*para*-Methoxyphenyl)-*4*-methyl-*1*-penten-*3*-one.
*alpha-alpha*-Dimethylanisalacetone.



$C_{13}H_{16}O_2 = 204.27$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Caramellic-fruity odor with a distinctly buttery topnote and good tenacity.

Sweet-caramellic taste with a fruity, berry-like note.

This ketone, the next higher homologue of the crystalline Ethone (see monograph: *alpha*-Methylanisal acetone), has been used in flavor compositions for many decades. It adds power and tart sweetness to berry flavors, a fruity note to Maple compositions, and it enriches a caramel flavor. Its comparatively high boiling point makes it a good fixative in flavors for baked goods, etc.

The concentration used is normally about 5 to 50 ppm in the finished product.

The subject material is occasionally used in perfume compositions as a modifier for the overly sweet fruity chemicals, Ethyl methyl phenyl glycidate, Ethyl phenyl glycidate, Undecanolide, etc. or for Palatone, Vanillin, Ethylvanillin, etc. in fruit complexes for top-notes or special effects in fragrances.

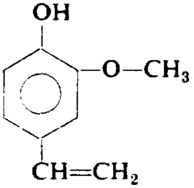
Prod.: by condensation of Anisaldehyde with Methyl-*iso*-propylketone.

G.R.A.S.

(Sample from Fritzsche Bros. Inc.).

## 1891: 2-METHOXY-4-VINYL PHENOL

*4*-Hydroxy-*3*-methoxy styrene.
*para*-Vinylguaiacol.
*iso*-Hesperitol.
*para*-Vinylcatechol-*ortho*-methylether.



$C_9H_{10}O_2 = 150.18$

Colorless or pale straw-colored oily liquid, solidifying in the cold. M.P. approximately 8° C. B.P. 224° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, spicy, Clove-like odor with a penetrating, warm, but also somewhat tarry undertone and good tenacity. It is considerably more diffusive than *iso*-Eugenol or Vanillin, but not quite as tenacious and not nearly as delicate.

This phenolether has found some use in flavor compositions, mainly in imitation Vanilla, Coffee, Cocoa, etc. where the power and radiation of the Aroma come to good effect.

The normal use concentration is equivalent to about 0.2 to 10 ppm in the finished product.

Probably on account of its comparatively high cost, this material is not used to any great extent in perfume compositions, where its effect can be simulated with lower cost Vanillin derivatives, Creosol, Eugenol derivatives, etc.

*4*-Vinylguaiacol produces Vanillin by oxidation.

Prod.:
1) by catalytic oxidation of *1,1*-Di-(*4*-hydroxy-*3*-methoxyphenyl)-ethane.
2) by decarboxylation of Ferulic acid.
3) The material may be present in Beechwood tar.

G.R.A.S. F.E.M.A. No.2675.

68-972; B-VI-954;

## 1892: METHYL ABIETATE

"Abalyn" (Hercules Powder Co.).
Abietic acid, methylester.
The commercial product consists of the mixed methylesters of the acids in Pine rosin (mostly Abietic acid).

$C_{21}H_{32}O_2 = 316.49$

Structure: see Abietic acid
Abitol
Hercolyn.

Almost colorless or pale straw-colored or pale amber-colored very viscous liquid.
Sp.Gr. 1.04. B.P. 365° C. (decompos.).

Insoluble in water, soluble in alcohol, but poorly soluble in diluted alcohol and Propylene glycol. Miscible with most oils.

Fresh batches may be almost odorless but carry a faint odor or acquire an increasingly perceptible, piney-woody odor of considerable tenacity and with a balsamic sweetness.

This material was developed for purposes other than perfumery, but it has found some use in perfume compositions as a fixative/blender, at times plainly as a diluent to reduce the overall cost of the fragrance product. Its comparatively large molecule is most conceivably responsible for the effect of reducing the odor level of fragrances in which Methyl abietate is incorporated.

It finds still some use in Pine fragrances, Lavender, Fougères, New Mown Hay, etc. but it can not be used in floral fragrances without a detrimental effect upon the floral theme.

A hydrogenated product, Hercolyn (see monograph) has largely replaced Abalyn as a perfume blender and low-cost fixative.

Prod.: from commercial Abietic acid by Methyl esterification.

26-596; 86-1; 86-88; 100-670; (Hercules Powder Co., special data sheet).

## 1893: METHYL ACETATE

Methyl ethanoate.
This is one of several products, occasionally sold under the name of "Acetone substitute".

$CH_3—COO—CH_3$

$C_3H_6O_2 = 74.08$

Colorless mobile liquid. B.P. 57° C.
Sp.Gr. 0.93.

25 % soluble in water, miscible with alcohol and oils.

Forms explosive vapor mixtures with air – fire hazard.

Sweet, and extremely diffusive, ethereal-fruity odor of very poor tenacity. In fact, one must hurry to smell it from a perfume blotter before it is completely evaporated.

This ester finds a little use in perfume compositions where it may give a much wanted "lift" to Citrus notes in Colognes, and make their alcoholic solutions smell "fresher" and "lighter". That type of Citrus-cologne topnote is not in high fashion in the United States of America, but it is occasionally called for in many other countries.

The ester is also sometimes applied to perfumes intended for products containing *iso*-Propyl alcohol, the penetrating topnote of which has a bad influence upon the performance of most fragrances. Traces of Methylacetate can temporarily distract the attention from the *iso*-Propylalcohol-note and carry the olfactory impression more swiftly over to the perfume.

Methylacetate is used in flavor compositions, mainly in Arak, Brandy, Rum, Whisky, fruit and Nut complexes, Raspberry imitation, etc. The concentration is normally about 0.1 up to 30 ppm in the finished product.

Prod.: by direct esterification of Methanol with Acetic acid or Acetic anhydride.

G.R.A.S. F.E.M.A. No.2676.

4-87; 26-596; 33-500; 86-88; 100-670; 103-80; B-II-124;

## 1894: METHYL ACETOACETATE

Methyl-*3*-oxobutanoate.
Methyl acetyl acetate.

$CH_3—CO—CH_2—COO—CH_3$

$C_5H_8O_3 = 116.12$

Colorless liquid. Sp.Gr. 1.08. B.P. 170 °C. (decomposes).

38 % soluble in water, miscible with alcohol and oils. Soluble in Propylene glycol and Glycerin.

Ethereal-green, winey odor of moderate to poor tenacity.

Sweet-ethereal, somewhat green-fruity, winey taste.

This ketoester has been suggested for use in flavor compositions as a modifier for the Ethylester (see Ethyl acetoacetate).

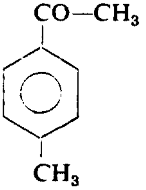
It does not fall quite so naturally into the winey or fruity flavor types most commonly called for, and it will most likely remain a small and rare ingredient.

Prod.:
1) from Methyl acetate and Sodium methoxide.
2) from Methanol and Diketen.

26-596; 66-873; 100-670; 160-776; B-III-632;

## 1895: para-METHYL ACETOPHENONE

*1*-Methyl-*4*-acetylbenzene.
*)Methylacetophenone.
Methyl-*para*-tolylketone.
*1*-Acetyl-*4*-methylbenzene.
*4*-Acetyltoluene.
Tolyl methyl ketone.
"Melilotal".
Melilot ketone.
"Melilone".
*) The commercial product is mainly: *-para-*.



$C_8H_{10}O = 134.18$

Colorless needles, or opaque, crystalline mass.
M.P. 28° C. B.P. 228° C. Sp.Gr. 1.00 (0.99 liquid).

Almost insoluble in water and Glycerin, soluble in alcohol, oils and Propylene glycol. Poorly soluble in mineral oil.

Pungent, almost harsh, but warm, sweet and floral odor of moderate tenacity. It resembles the odor of Acetophenone but is not nearly as agressive or harsh-gassy. The Methyl-derivative is more fruity in the direction of Methylbenzoate, and deep-sweet as Hydroquinone dimethylether.

Although it is repeatedly classified as a Mimosa-type odor, this description should not be taken too literally. In compositions, however, the material may produce floral notes and contribute to the picture of Mimosa.

Sweet, woody-floral taste, only in extreme dilution becoming fruity, vaguely reminiscent of Strawberry (but Ethyl-acetophenone is far superior in that respect).

The coumarinic-Hay-like or Bitter-Almond-like notes are utilized in perfume compositions for herbaceous notes, Fougères, New Mown Hay, Lavender, Mimosa, Acacia, Chypre, Hawthorn, etc. It blends excellently with Anisaldehyde, Coumarin, Heliotropine, etc. all of which help make the subject ketone sweeter and less harsh, at the same time utilizing the power and radiance of the ketone.

It finds some use in flavor compositions for imitation Almond, Vanilla and various fruit complexes.

The normal concentration is about 1 to 10 ppm but may be as high as 500 or 1,000 ppm in chewing gum.

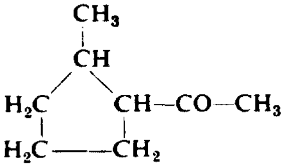
Prod.: by Friedel-Craft's reaction upon Toluene, Acetic anhydride and Aluminum chloride.

G.R.A.S. F.E.M.A. No.2677.

7-267; 26-598; 31-83; 34-679; 68-532; 86-88; 89-458; 88-391; 4-87; 95-170; 103-152; 103-270; 106-237; 160-782; B-VII-307;

## 1896: METHYL ACETYL CYCLOPENTANE

*2*-Acetyl-*1*-methylcyclopentane.



$C_8H_{14}O = 126.20$

Colorless mobile liquid. The *trans*-form is the stable form. B.P. 168° C.

Almost insoluble in water, soluble in alcohol and oils.

Ethereal, warm-herbaceous odor of poor tenacity.

This ketone has found some use in perfume compositions, mainly for its power and low cost, but also for its ability to enhance pungent floral odors, e. g. Jasmin, Wallflower, Wistaria, and certain herbaceous fragrances, e. g. New Mown Hay, etc.

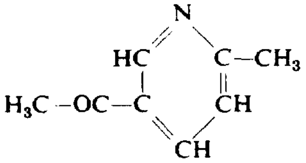
It is interesting to notice the similarity of this molecule to that of Methylacetophenone, Acetylcyclohexane, etc. – see these monographs.

Prod.: from Cyclohexane plus Acetylchloride and Aluminumchloride.

3-171; 67-109;

## 1897: 2-METHYL-5-ACETYL PYRIDINE

*5*-Acetyl-*2*-picoline.
*5*-Methyl-*2*-picolinyl ketone.



$C_8H_9NO = 135.17$

Pale yellowish or pale lemon-yellow, oily liquid.

Practically insoluble in water (soluble in aqueous alkali), soluble in alcohol and oils.

Powerful, sweet but somewhat choking odor when undiluted, sweet, almost floral, yet heavy in extreme dilution.

This Pyridine ketone has been suggested for use in certain floral bases and artificial flower absolutes for its powerful notes, imitating those of Jasmin, Tuberose, Tobaccoflower, etc.

Many derivatives of Pyridine and Piperidine are used in trace amounts in floral bases, and Pyridine itself is approved for use in flavor compositions (G.R.A.S.). However, the perfumers generally have a reluctance in using chemicals with names indicating any relationship to Nicotine, Pyridine, Cyanide, etc. partly for psychological reasons, partly because many members of those chemical families are toxic or otherwise hazardous.

Modern perfumers are probably more inclined to use chemicals with less fear of their alarming names, and it is most conceivable that many Pyridine derivatives can be used safely in the concentrations required – which is very, very low.

Prod.: from coal tar; along with Pyridine is obtained Picoline which is treated with Lithium and reacted with Acetic anhydride to acetylate the *2*-Picolyl lithium.

See also: 69-554; 86-4; 86-89;

## 1898: METHYL ALCOHOL

Methanol.
Wood spirits.
Carbinol.
Wood alcohol.

$CH_3—OH$

$CH_4O = 32.04$

Colorless mobile liquid. Sp.Gr. 0.79. B.P. 65° C.

Miscible with water, alcohol, Propylene glycol, Glycerin and oils. Its vapors may form explosive and flammable mixtures with air at room temperature.

Very pure Methyl alcohol has only a mild odor, but commercial grade Methylalcohol will usually display a somewhat pungent-gassy topnote followed by a sweeter ethereal odor of very poor tenacity.

This alcohol is rarely used as such in perfumes, but it finds use as a solvent for extraction of plant material, Resins, etc. for the production of Resinoids, Concretes, etc. in perfumery.

It is also used as a denaturant in Ethylalcohol for use as a perfume extraction solvent. The American "Specially Denatured Alcohol" No. 30 contains 10% Methanol in Ethanol, while No. 3A contains 5% Methanol. There is therefore always traces of Methanol present in extracts made with these solvents.

Since Methanol occurs in Pectin, free and combined, it is also a component of many fruit juices and in Tobacco smoke.

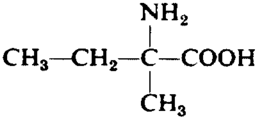
Methanol is not used in flavors. It is considered moderately toxic, and doses of 25 grams or more may be fatal to adult human beings.

Prod.: from Hydrogen plus Carbon monoxide or dioxide. It is also produced by oxidation of hydrocarbons.

26-598; 34-806; 66-297; 77-167; 85-85; 100-664; 160-1098; B-I-273;

## 1899: alpha-**METHYL**-alpha-**AMINOBUTYRIC ACID**

*D,L-iso*-Valine.
*dl-2*-Amino-2-methylbutanoic acid.



$$CH_3-CH_2-\overset{\displaystyle NH_2}{\underset{\displaystyle CH_3}{C}}-COOH$$

$C_5H_{11}NO_2 = 117.15$

Colorless or white prismatic crystals.
M.P. 308° C. (decomposes). The material sublimes below the melting point.

30% soluble in water, 6% soluble in hot alcohol, poorly soluble in cold alcohol, soluble in most oils.

This material has only a very faint odor, and is probably odorless when absolutely pure. Its taste is bland, sometimes described as "broth-like", but weak.

The acid as such is not extensively used in flavors, but it plays an important role as a "precursor" for flavors in dairy products, meats and fruits. It is found widely distributed in natural products, and modern flavor technology takes advantage of the knowledge of its existence and role in those products.

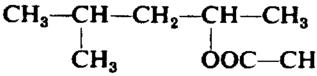
Secondary flavor products are prepared from the acid through a great variety of reactions, some of which simulate the reactions that presumably take place in Nature.

Isomers and derivatives of the acid are found in products as different as Roquefort cheese and Bananas, but it is an established fact that the acid is not contributing to the typical flavor of Roquefort cheese or Banana. However, it does form a characteristic "background" flavor in all such products, and without this background flavor it is simply not possible to approach the natural flavor by imitation.

61-54; 100-582; 117-59; 160-1068;

## 1900: METHYL AMYLACETATE

Methyl-*iso*-butyl carbinylacetate.
(An *iso*-Hexylacetate).



$$CH_3-\underset{\displaystyle CH_3}{CH}-CH_2-\underset{\displaystyle OOC-CH_3}{CH}-CH_3$$

$C_8H_{16}O_2 = 144.22$

Colorless oily liquid. Sp.Gr. 0.86.

Almost insoluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Mild and pleasant fruity odor, sweeter than *iso*-Amylacetate, less Pear-like, more Banana-like, moderate to poor tenacity.

Sweet fruity, Banana-like taste with a Raspberry-like note.

This ester is only rarely used in perfumes, but it finds some application as a masking agent in industrial fragrances, masking odors, etc.

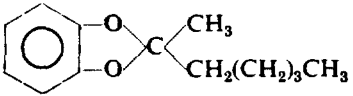
It is also used in flavor compositions for its versatile fruity character in Raspberry imitation, Banana, Pineapple, Pear, Apple, and in "Tutti-frutti" or "Juicy-fruit" type flavors.

Prod.: by direct esterification of Methyl-*iso*-butylcarbinol with Acetic acid or Acetic anhydride.

30-206;
(sample: Union Carbide Chemicals Co.).

## 1901: METHYL AMYL CATECHOL KETAL

Pyrocatechol methylamyl ketal.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid.

Fruity-herbaceous, but somewhat harsh, Jasmin-like odor of good tenacity.

This ketal, although rarely offered commercially, is manufactured by a number of creative perfume houses for "captive" use in various fragrances.

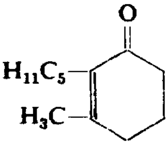
It lends power and novel notes to Jasmin compositions, and it can be used in general as a floralizer/blender with some fixative value.

It forms member of a series of ketals produced from symmetric and asymmetric alifatic ketones with Catechol (Pyrocatechin). A number of these ketals have interesting floral odors.

Prod.: by condensation of Catechol with Methyl amyl ketone.

30-253; 31-118; 31-117; 159-416;

## 1902: 5-METHYL-6-AMYL-5-CYCLOHEXEN-1-ONE



$C_{12}H_{20}O = 180.29$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, but rather dry, floral odor of good tenacity. The floral notes are most perceptible in actual use, while the material per se displays a non-descript, slightly green-woody floralcy.

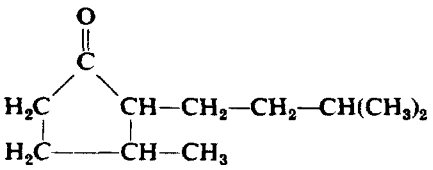
With proper blending, this ketone can lend useful and attractive power and background to a great variety of odor types. It blends well with the Ionones, Amylsalicylate, Cyclamen-aldehyde, Linalool, Ambre-materials, etc.

The title material represents an extensive series of new fragrance chemicals developed from Tetrahydrobenzaldehyde or Cyclohexenone by di-alkyl substitution.

(See American Perfumer & Cosmetics, Vol. 83, April 1968, page 31).

## 1903: 3-METHYL-2-iso-AMYL CYCLOPENTANONE

A Tetrahydrojasmone.



$C_{11}H_{20}O = 168.28$

Colorless or pale straw-colored oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, floral-fruity, Jasmin-like odor of good tenacity and considerable radiation. Many perfumers consider this ketone superior to the *n*-Amyl derivative.

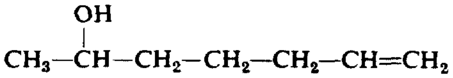
It finds some use in perfume compositions as a floralizer and intensifier of existing floral notes. It is used not only in Jasmin compositions, but also in Tuberose, Neroli, Lilac and many other florals as well as in a number of non-floral types.

Prod.: from *omega*-Methyl-*2,5-gamma*-undecan dione.

5-154; 86-94; see also: 156-223;

## 1904: METHYL-delta-AMYLENYLCARBINOL

Methyl-*4*-pentenylcarbinol.
*2*-Hydroxy-*6*-heptene.



$CH_3-\overset{\overset{OH}{|}}{C}H-CH_2-CH_2-CH_2-CH=CH_2$

$C_7H_{14}O = 114.19$

Colorless liquid.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Peculiar Incense-like, resinous odor of moderate to poor tenacity.

This alcohol, rarely offered commercially, has been suggested for use in perfume compositions.

It offers a rare type of odor, only occasionally needed. But it gives pleasant effects with Olibanum and Opopanax, with Elemi, etc. and with the herbaceous oils, Lavender, Lavandin, etc.

If it were freely available at low cost, it could undoubtedly be used in modern soap perfumes of woody, fresh-aldehydic type, or the slightly medicated type.

Prod.: (several methods) e. g. from Allylacetic ester by reduction to *4*-Pentenol, which is oxidized to *4*-Pentenal. The aldehyde gives the title alcohol via Grignard reaction with Methyl magnesium iodide.

3-175; 163-102;

## 1905: METHYL-n-AMYLKETONE

Amyl methyl ketone.
*2*-Heptanone.
Ketone C-*7*.

$CH_3-CO-(CH_2)_4-CH_3$

$C_7H_{14}O = 114.19$

Colorless liquid. Sp.Gr. 0.81. B.P. 152° C.

0.4% soluble in water, miscible with alcohol and oils, soluble in Propylene glycol. The ketone will dissolve 1.4% water.

Penetrating, fruity-spicy light and volatile odor with resemblance to the fresher notes in Cinnamon bark. However, it is generally classified as a rather "chemical" odor, and only in extreme dilution it displays the more attractive spicy fragrance.

At concentrations below 50 ppm the taste is fresh, creamy-spicy, slightly fruity.

The ketone finds application in perfume compositions as a minor ingredient in Carnation or other spicy fragrances, in herbaceous types along with Estragon or Basil or Hyssop oils, and generally as a novel type of fresh topnote. It blends well with spicy and fruity fragrance materials. .

In flavors, it may add the "bite" to a Roquefort cheese flavor, or the fruity creamy note to a Banana flavor. It is also used in Coconut, Butter, various berry complexes, cheese and fruit blends, etc.

The normal use concentration is equivalent to about 2 to 25 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2544.

Prod.:

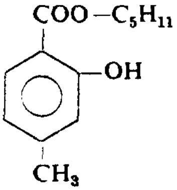
1) from Ethyl butyl acetoacetate.
2) from Heptyne by hydration.

4-87; 26-598; 31-80; 66-516; 77-210; 86-89; 89-166; 100-513; 160-1028; B-I-699;

## 1906: METHYL AMYL SALICYLATE

*para*-Methyl amylsalicylate.
Amyl-*meta*-cresotinate.
Amyl-2-hydroxy-*para*-toluate.
Amyl-*para*-methylsalicylate.

The chemical, sold under this name has occasionally been referred to in perfumery literature as:
*ortho*-Methoxy amylbenzoate,
but the author believes that the chemical originally sold under the title name was the -cresotinate.



$C_{13}H_{18}O_3 = 222.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous odor with a deep floral undertone and a trace of a fruity character.

This ester has been used in floral perfume compositions of the heavy-"exotic" character, and in Fougères as a modifier for the conventional Salicylates. It is more powerful and volatile than Amylsalicylate, not as pungent as Methylsalicylate, but it has overall more versatility than the two. Its hydroxyl radicle carries with it the usual disadvantages of a phenol in perfumery.

The ester is rarely offered under its proper chemical name, and the name itself causes quite some confusion as to the identity of the material.

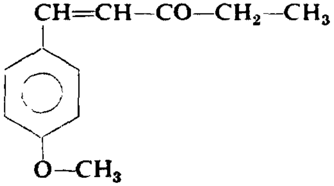
The *para*-Methyl methylsalicylate is also used in perfumery, see monograph under that name.

Prod.: from Ethylacetoacetate plus Aceto acetaldehyde, followed by esterification with Amylalcohol.

3-77; 4-87; 3-85;
see also: 68-770;

## 1907: alpha-METHYL ANISALACETONE

*alpha*-Methyl anisylidene acetone.
*1-para*-Methoxyphenyl penten-*1*-one-*3*.
*para*-Methoxystyryl ethylketone.
"Ethone" (Givaudan).
Anisylidene methyl ethyl ketone.



$C_{12}H_{14}O_2 = 190.24$

White or cream-colored or ivory-colored crystals. M.P. 60° C.

Practically insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Buttery-caramellic, sweet and lasting odor. Develops a somewhat sharp or pungent top-note upon storage.

Sweet-caramellic taste with a slightly fruity undertone. Slightly burning sensation at concentrations higher than 50 ppm.

This material finds only a little use in perfumes where its peculiar odor is rarely called for. Certain floral bases can benefit from the creamy notes, simulating the oily-buttery odor from flower petals, e. g. Tuberose and Ylang-Ylang.

The ketone is more frequently used in flavor compositions, particularly in imitation Maple, Caramel, Butter, Butterscotch, Rum and a few types of berry flavor, where the mild "bite" of this material may be desirable, e. g. Blackcurrant. It is also used in trace amounts in Vanilla, Nut, Cream and in various fruit complexes.

The concentration varies from 2 to 30 ppm in the finished product.

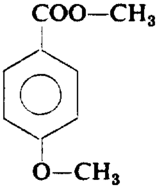
G.R.A.S. F.E.M.A. No.2673.

Prod.: by condensation of Anisaldehyde with Methyl ethyl ketone.

4-87; 41-122; 86-88; 106-143; 86-51;

## 1908: METHYL ANISATE

*para*-Methoxy methylbenzoate.
Methyl-*para*-methoxybenzoate.



$C_9H_{10}O_3 = 166.18$

White crystals. M.P. 48° C. B.P. 256° C.

Practically insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Sweet-herbaceous, delicately floral odor of good tenacity. It bears some resemblance to Lilac, Lindenblossom and Magnolia.

Sweet-herbaceous taste reminiscent of Chervil-salad, slightly spicy-green. Anise-like at higher concentrations.

This ester finds some use in perfume compositions as a sweetener and floralizer in Lilac, Mimosa, Hawthorne, Sweet Pea, Freesia, Magnolia, Lindenblossom, etc. It supports the fixation and lends a nondescript sweetness when used in discrete amounts. Overdoses will usually show up as "anisic" and generally undesirable effects.

It is used in flavor compositions for imitation Melon, Vanilla, and in Anise-Menthol complexes for licorice flavoring, in fruit complexes, liqueur flavors, root-beer flavor and various spice blends.

The concentration is about 2 to 10 ppm in the finished product.

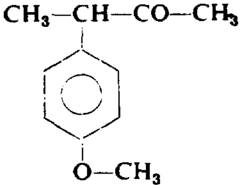
G.R.A.S. F.E.M.A. No.2679.

Prod.: by direct esterification of *para*-Anisic acid with Methylalcohol e. g. under azeotropic conditions.

4-87; 26-608; 31-160; 34-680; 86-89; 103-83; 106-238; 160-806; B-X-159;

## 1909: alpha-METHYL ANISYL KETONE

2-(*para*-Methoxyphenyl)butan-*3*-one.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid. B.P. 260° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and somewhat woody-floral odor of rather nondescript character, vaguely reminiscent of Rose, but with a chemical-woody undertone and considerable tenacity.

Subject material has been suggested for use in perfume compositions as a modifier in woody-floral soap perfumes on account of its stability and good tenacity.

The author has chosen to use the commercial name "*alpha*-Methyl anisyl ketone" as head name for this monograph, although the description actually refers to 2-(*para*-Methoxyphenyl)butan-*3*-one, which is an isomer of the well-known "*para*-Methoxyphenylbutanone" (see monograph of that name).

Perfumery literature is notoriously plagued with misleading chemical names and confusing nomenclature, and it is one of the objects of this work to minimize such errors and confusion.

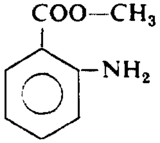
The title name of this monograph is admittedly confusing, and it may well refer to the named isomer or to an entirely different chemical.

The subject material (synonym name) is produced from *alpha-alpha*-Dimethyl-*alpha*'-*para*-methoxyphenylethylene oxide. It can also be prepared from the corresponding glycol.

4-49; 68-752; see also No. 1907.

## 1910: METHYL ANTHRANILATE

Methyl-*2*-aminobenzoate.
*ortho*-Amino methylbenzoate.



$C_8H_9NO_2 = 151.17$

Colorless liquid or white to pale straw-colored crystalline mass, or white crystals (highly purified material). M.P. 24° C. B.P. 237° C. Sp.Gr. 1.17 (liquid).

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils, almost insoluble in Glycerin.

Musty-fruity and somewhat dry-floral odor reminiscent of Concord grapes, Orangeblossom, and having good tenacity. The odor appears much sweeter in high dilution.

Sweet fruity, Grape-like taste with a distinctly floral-perfumey character.

This ester is widely used in perfume compositions as a sweet-floral Orangeblossom-type ingredient. Often applied in combination with Petitgrain oil, it supplies much of the background in Cashmere bouquet type fragrances and other Oriental, heavy floral or sweet-woody types. Its condensation products with various aldehydes (Schiff's bases) or with Acetophenone, Musk Ketone, Ionones, etc. are often utilized in perfume compositions. It should therefore be kept in mind that when Methylanthranilate is used in compositions with one or more of the named (or other) aldehydes and ketones, there is a good chance of chemical processes taking place in the perfume oil. The change may be visually perceptible (color increases, usually to yellow or browninsh tints) or olfactory (intensified sweetness, loss of aldehyde components etc.) and it may take place over a period of from 24 hours up to many months.

Completed condensation products (Schiff's bases, etc.) are often preferred to avoid such annoying changes in the perfume, rarely understood by the customer.

The most popular condensation products are those with the floral aldehydes: Hydroxycitronellal (Aurantiol, etc.), Anisaldehyde (Acaciol), etc. Certain aldehydes produce very dark colored condensation products and should be avoided in compositions where Methyl anthranilate must be used (Citral, Citronellal, etc.). When the two components enter at very low percentage, there is generally no discoloration problem (several Citrus oils contain Citral and Methyl anthranilate at the same time).

The ester finds also extensive use in flavor compositions, not only in Grape (to imitate the Concord Grape in which it is a natural component), but also in various berry flavors, Melon, Honey, Citrusfruit, floral types (Rose-Violet, etc.) wine, liqueur, etc.

The concentration may be as low as 0.2 ppm in liqueurs, where the addition must be extremely discrete, or 20 to 50 ppm in candy and various other consumer products. In chewing gum it is occasionally used at concentrations up to 2,200 ppm (or one part of the ester in 450 parts of chewing gum). This is equivalent to 22% of Methylanthranilate in a flavor used at 1% in the chewing gum.

G.R.A.S. F.E.M.A. No.2682.

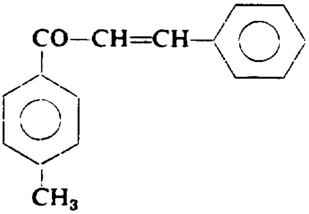
Prod.:

1) by direct esterification of Anthranilic acid with Methanol e. g. under azeotropic conditions.
2) from Isatoic anhydride with Methanol and Sodium methylate.

4-87; 5-289; 26-598; 34-1011; 68-578; 85-28; 86-89; 77-213; 90-795; 95-189; 96-216; 100-672; 103-83; 106-239; 160-810; B-XIV-317;

## 1911: para-METHYL BENZALACETOPHENONE

Benzylidene-*para*-methylacetophenone.



$C_{16}H_{14}O = 222.29$

Colorless viscous liquid, solifying in the cold.

Insoluble in water, soluble in alcohol and oils.

Warm and sweet, deep-floral, heavy odor, reminiscent of exotic flowers, Tuberose, Gardenia, etc. and with a remote resemblance to refined Labdanum.

This ketone has been suggested for use in perfume compositions, but it is rarely offered commercially under its proper name. There has also been some confusion with Dypnon, which is Methyl-7-benzalacetophenone.

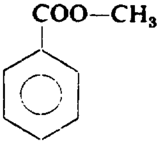
The subject material could find some use in perfumes and floral bases, such as Mimosa, Tuberose, Gardenia, Honeysuckle, Orange-blossom, etc. and as a fixative in many other heavy floral types, Oriental fragrances, etc.

Prod.: by condensation of *para*-Methylacetophenone with Benzaldehyde.

31-84; 7-270;

## 1912: METHYL BENZOATE

"Niobe oil".



$C_8H_8O_2 = 136.15$

Colorless liquid. Sp.Gr. 1.09. B.P. 200° C.

0.02% soluble in water, soluble in alcohol, Propylene glycol and oils. Almost insoluble in Glycerin.

Pungent, heavy-sweet, deep-floral odor of moderate to poor tenacity. Its fruity undertones resemble Prunes and Blackcurrant, while the heavy floral tones recall notes of Tuberose or Longoza.

Sweet, berry-like, somewhat spicy, slightly Nutmeg-like taste in dilutions below 20 ppm. Pungent at higher concentrations.

This ester is widely used in perfume compositions and floral bases. It is a conventional ingredient in "Peau d'Espagne" and in Ylang-Ylang bases, it is used for its low cost in detergent fragrances, masking odors and industrial perfumes. It blends excellently with Benzyl acetate, Cinnamic alcohol, Cresylethers and esters, Methylanthranilate, etc. and with most of the spice oils.

The ester is also extensively used in flavor compositions for imitation Strawberry, Raspberry, Pineapple, Rum, Vanilla, and in fruit complexes, liqueur flavors, Nut flavors, etc.

The normal concentration is about 2 to 10 ppm in the finished product.

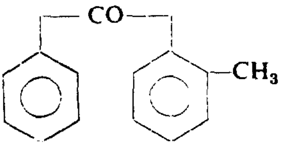
G.R.A.S. F.E.M.A. No.2683.
FCC-1964-855.

Prod.: by direct esterification of Benzoic acid with Methanol, preferably using azeotropic conditions. The esterification takes place so readily, that heating of the two components will cause formation of perceptible amounts of the ester. This esterification may take place when Benzoin Siam is heated with denatured alcohol in the preparation of Benzoin resinoid. The resinoid contains accordingly measurable amounts of Ethyl- and Methyl benzoate, not originally present in the crude natural material.

4-88; 26-600; 68-546; 77-192; 85-85; 86-89; 90-326; 100-672; 103-82; 106-241; 160-850; B-IX-109;

## 1913: ortho-METHYL BENZOPHENONE

2-Methyl benzophenone.
Phenyl-*ortho*-tolylketone.



$C_{14}H_{12}O = 196.25$

Colorless viscous liquid. B.P. 315° C.

Solidifies in the cold.

Very faint odor, remotely rosy, sweet, musty. Overall softer and perhaps even weaker than Benzophenone.

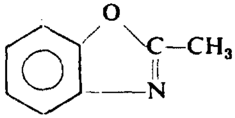
This ketone has been suggested for use in perfume compositions as a fixative/blender. It does not offer any advantages over Benzophenone in this respect, and it is rarely available at the same low cost as Benzophenone. It displays its proper odor more perceptibly when it is combined with more volatile components, and in that respect it also resembles Benzophenone.

Prod.: by condensation of Benzoyl chloride and Toluene with Aluminum chloride and a catalyst.

68-1063;
(sample: Norda Ess. Oil & Co.).

## 1914: 2-METHYL BENZOXAZOLE

Ethenyl aminophenol.



$C_8H_7NO = 133.15$

Yellowish liquid, solidifying in the cold.
M.P. 10° C. Sp.Gr. 1.13. B.P. 201° C.

Insoluble in water, soluble in alcohol, miscible with most oils.

Very sweet odor of rather gassy-pungent character when undiluted, becoming floral-sweet, heavy, when diluted.

This material has been suggested for use in perfume compositions as a powerful ingredient in various floral and sweet-Oriental or tobacco-woody fragrance types. For academic reasons, the relationship to Skatole is of some interest, particularly in the study of the influence of an Oxygen atom in the heterocyclic portion of the molecule.

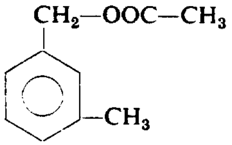
The subject material suffers from being rather unstable under acid conditions and under heat by which it decomposes.

Prod.: from *ortho*-Aminophenol plus Acetic anhydride by heating and distilling.

26-538; 69-376; 160-864; B-XXVII-46; 163-358;

## 1915: METHYL BENZYL ACETATE

The commercial material consists mainly of *meta*-Methyl benzyl acetate.
This is not identical to the more common material known as: *para*-Tolyl acetate (see that monograph).
*3*-Methyl benzyl acetate.
*meta*-Tolyl carbinyl acetate.



$C_{10}H_{12}O_2$ = 164.21

Colorless liquid. B.P, 217° C. Sp.G. 1.04.

Almost insoluble in water, soluble in alcohol and oils.

Powerful fruity and intensely sweet odor of moderate to poor tenacity. The fruity notes resemble Cherry – milder and sweeter, less pungent than Benzyl acetate, also less floral.

Sweet fruity taste reminiscent of Banana and Cherry.

This material is mainly used in flavor compositions (the *para*-isomer is more commonly used in perfumes).

It finds application in imitation Cherry, Pear, Banana and other fruits, in "Tutti-frutti" and other fruit complexes, etc.

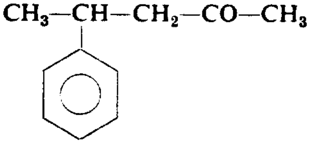
The normal concentration is about 1 to 10 ppm, but it may be as high as 200 ppm in chewing gum (e. g. "juicy-fruit" type gum).

Prod.: from *meta*-Tolylchloride (which contains some *para*-isomer) with aqueous alkali under reflux, followed by esterification of the alcohol.

(See also 68-499).

## 1916: alpha-METHYL BENZYL ACETONE

*1*-Methyl-*1*-phenylbutanone-*3*.
*4*-Methyl-*4*-phenyl-*2*-butanone.
*2*-Phenylpentan-*4*-one.



$C_{11}H_{14}O$ = 162.23

Colorless oily liquid. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet woody, somewhat spicy and warm odor of moderate tenacity. It has undertones sometimes described as fruity, but they are not accompanied by the sweetness found in e.g. *para*-Methoxyphenylbutanone or similar materials.

This ketone has been suggested for use in perfume compositions as a modifier for the conventional floral-woody chemicals, the "rose" alcohols, etc. and it blends rather well with the Ionones, Cedarwood derivatives, Heliotropine, Amylsalicylate, etc.

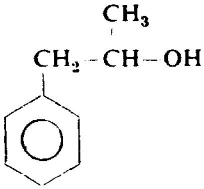
It is not commonly available under its proper chemical name, and rarely found on the perfumer's shelf.

Prod.: by rearrangement of *1*-Methyl-*1*-phenylbutane-*1,2*-diol.

68-540; see also 1706.

## 1917: METHYL BENZYL CARBINOL

Benzyl methyl carbinol.
*1*-Phenylpropan-*2*-ol.
*alpha*-Methyl-*beta*-phenylethyl alcohol.
Exists in *d*-, *l*- and *dl*-forms.



$C_9H_{12}O = 136.20$

Colorless liquid. B.P. 220° C. Sp.Gr. 1.00.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and somewhat floral-green odor with a Honey-like undertone and moderate to poor tenacity.

Although this carbinol is one of the simplest and most accessible of several dozens of perfumery carbinols, it has never achieved much popularity or aroused interest. It could find use in Lilac and Hyacinth type fragrances and it could be used as a modifier in Rose compositions, particularly for soap.

The next higher homologue, Dimethyl benzyl carbinol is one of the most popular members of the series.

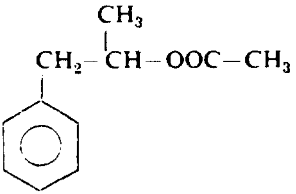
Prod.:

1) by reduction of Phenylacetone with Sodium in boiling alcohol (produces mainly the *racemic*-form).
2) by hydrogenation of Methyl benzyl ketone.
3) from Styrene oxide and Methyl magnesium bromide by Grignard type reaction.

4-88; 5-71; 68-500; 86-90; 103-291; 37-513; 37-515;

## 1918: METHYL BENZYL CARBINYL ACETATE

*alpha*-Methyl-*beta*-phenylethyl acetate.
Benzyl methyl carbinyl acetate.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. B.P. 225° C. Sp.Gr. 1.01.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-floral, slightly green and fruity odor with a Hyacinth-like note, remotely resembling that of Hydratropyl acetate.

In spite of being the next lower homologue of one of the most widely used perfumery carbinyl acetates, this ester has found very little interest in the perfume world.

It could be used as a modifier in many floral or Oriental fragrance types, in Fougères, etc. if it were as commonly available and lower priced than its "big" brother (D.M.B.C.A.).

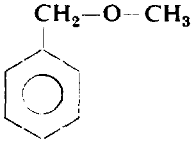
It is stable in soap and it is actually extremely versatile in its use, from distinctly floral to strictly herbaceous or green.

Prod.: by direct esterification of the carbinol with Acetic acid e. g. under azeotropic conditions.

4-88; 37-516; 86-90;

## 1919: METHYL BENZYL ETHER

Benzyl methyl ether.



$C_8H_{10}O = 122.17$

Colorless liquid. Sp.Gr. 0.98. B.P. 171° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar, rather sharp-metallic, fruity-rosy odor of poor tenacity.

This ether is occasionally used in soap perfumes, industrial perfumes and masking odors, where power and low cost are essential.

It lends more diffusive power than Diphenyl oxide or Diphenyl methane, but not as much tenacity. It is stronger smelling than Methyl diphenylether, but also harsher.

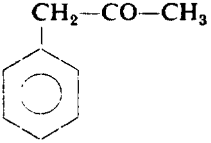
This material does not seem to have much future in perfumery.

Prod.: from Benzyl chloride and Sodium methoxide in Methanol solution.

37-171; 68-502;

## 1920: METHYL BENZYL KETONE

Benzyl methyl ketone.
Phenylacetone.
*3*-Phenyl-*2*-propanone.



$C_9H_{10}O = 134.18$

Colorless liquid. B.P. 215° C. Sp.Gr. 1.01.

Almost insoluble in water, soluble in alcohol and oils.

Green, rather sharp and unnatural odor of moderate to poor tenacity. The odor bears some similarity to that of *para*-Cresol ethyl ether, but is not quite as floral.

This ketone has been suggested for use in perfume compositions, but does not seem to have any significant fragrance value or any outstanding olfactory properties. It could find some use in Narcissus, Jasmin or various floral bouquets for low-cost fragrances, where power and stability is important.

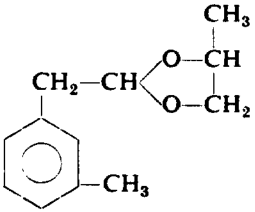
To the author's knowledge, this material is rarely used in perfumes.

Prod.: by hydrolysis of *alpha*-Phenylaceto acetonitrile or from Acetic acid plus Phenylacetic acid vapors over a heated catalyst.

4-114; 36-1251; 68-538; 86-90;

## 1921: 1-meta-METHYL BENZYL-4-METHYL-1,3-DIOXOLAN

"Tolylaldehyde Propyleneglycol cyclic acetal".
*5*-Methyl-*2*-*meta*-tolyl-*1*,*3*-dioxolane (correct name).



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid.

Slightly soluble in water, soluble in alcohol and oils, slightly soluble in Propylene glycol.

Sweet floral-herbaceous and quite lasting odor, remotely reminiscent of Lilac. The sweetness resembles Anise and Vanilla.

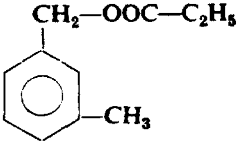
This cyclic acetal has been suggested for use in perfume and flavor compositions, but it is very rarely offered under its chemical name. Several commercial specialties and bases contain this chemical as a major ingredient. Since the commercial chemical inevitably contains considerable amounts of *para*-isomer and perhaps other isomers, a general odor description is of little value without the material in hand.

The literature reveals that series of cyclic acetals have been prepared experimentally from time to time over many decades, but only a few of these acetals have achieved a permanent place on the perfumer's or flavorist's shelf.

Prod.: by condensation of Propyleneglycol with *meta*-Tolylacetaldehyde (*meta*-Methyl phenylacetaldehyde).

(See also: 31-73). See monograph 2874.

## 1922: meta-METHYL BENZYL PROPIONATE



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid. B.P. 230° C.

Insoluble in water, soluble in alcohol and oils.

Warm and sweet, deep-floral, slightly fruity odor of moderate tenacity.

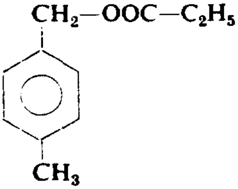
This ester, not a very common perfume material, is occasionally used as a modifier for the heavy floral esters in Ylang-Ylang, Narcisse, Hyacinth and other pungent florals. It is somewhat more fruity than Methyl-*para*-toluate, a more common member of the family, but it is also less "anisic" in its character.

Prod.: by direct esterification of *meta*-Tolylalchohol with Propionic acid.

68-544; 160-1254;

## 1923: para-METHYL BENZYLPROPIONATE

*para*-Tolyl propionate.
*para*-Cresyl propionate (confusing name).



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet, fruity-floral odor of moderate tenacity. The fruity notes are less pronounced, the sweet-floral notes more pronounced than in Benzylpropionate.

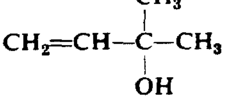
This material would primarily act as a sweetener, and it has interesting effect in Jasmin compositions, Gardenia, floral bouquets, etc. where effects of longer duration than those offered by Benzylacetate, are desirable.

The material is not specifically listed as G.R.A.S. in the authoritative American lists, but it could find use in Pear and "Tutti-frutti" flavor compositions in areas where its use is not banned.

Prod.: by direct esterification of *para*-Tolylalcohol with Propionic acid or Propionic anhydride.

## 1924: 2-METHYL-3-BUTEN-2-OL

Dimethyl vinylcarbinol.
(An *iso*-Pentenol).



$$CH_2{=}CH{-}\underset{OH}{\overset{CH_3}{C}}{-}CH_3$$

$C_5H_{10}O = 86.14$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, oily-herbaceous, somewhat earthy, fungus-like odor of considerable radiance. Poor tenacity.

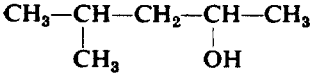
This unsaturated alcohol has found a little use in perfume compositions, mainly in the reconstruction of Lavender and Lavandin oils, etc. It is occasionally used as a powerful additive in soap and detergent perfumes, but it needs skilful blending and firm fixation in order to control its odor to an acceptable level.

Prod.: from Vinyl magnesium bromide and Acetone by Grignard reaction.

Se also: Pentenol and Prenol.

## 1925: METHYL-iso-BUTYLCARBINOL

Methyl amylalcohol.
4-Methyl-2-pentanol.
(An *iso*-Hexanol).



$$\underset{\displaystyle CH_3}{CH_3{-}\overset{}{CH}}{-}CH_2{-}\underset{\displaystyle OH}{CH}{-}CH_3$$

$C_6H_{14}O = 102.18$

Colorless liquid. B.P. 132° C. Sp.Gr. 0.81.

1.7% soluble in water, miscible with alcohol and oils, soluble in Propylene glycol. It will dissolve 6% water at room temperature.

Powerful oily-green somewhat herbaceous, but overall "chemical" or "un-natural" odor of poor tenacity. Repeated inhalation of its vapors cause coughing.

This alcohol is used very rarely as such in perfumery, but its derivatives, esters, etc. are used more widely.

The alcohol itself finds some application as a masking agent on account of its low boiling point and availability in volume at low cost.

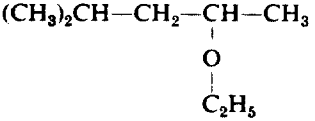
Prod.: by hydrogenation of Methyl-*iso*-butylketone. (See that monograph).

(Union Carbide Chemical Co. data sheet).

The acetate of this alcohol is listed under: Methyl amylacetate.

## 1926: METHYL-iso-BUTYLCARBINYL ETHYLETHER

Ethyl-*iso*-hexylether.
*iso*-Hexyl ethylether.



$$(CH_3)_2CH{-}CH_2{-}\underset{\displaystyle \underset{\displaystyle C_2H_5}{O}}{CH}{-}CH_3$$

$C_8H_{18}O = 130.23$

Colorless mobile liquid. B.P. 137° C.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

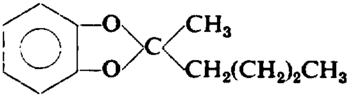
Refreshing, green-ethereal, herbaceous-fruity odor of poor tenacity.

This ether has found occasional use in perfumery, mainly as a trace component in certain floral fragrances, as a "lift" to Lavender and Geranium, but also in larger amounts as a masking ingredient in industrial fragrances, where diffusive power and low cost are the prerequisites in many cases.

Prod.: from Methyl-*iso*-butylcarbinol plus Ethanol by dehydration.

## 1927: METHYL BUTYL CATECHOL KETAL

Pyrocatechin methyl-*n*-butylketal.
Catechol methyl butyl ketal.



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Somewhat sharp-floral, Jasmin-like fruity odor of good tenacity.

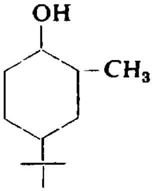
This ketal, a member of a long series of Catechol condensation products with alifatic symmetric and asymmetric ketones, has been suggested for use in perfume compositions on account of its floral odor and a tenacity which is superior to most materials with a similar odor.

It is rarely offered under its proper chemical name, and apparently only manufactured on a "private" scale by the few fragrance houses using it. Overall it does not seem to offer any significant advantage over the conventional and easily accessible Jasmin-floral materials.

Prod.: by condensation of Methyl-*n*-butylketone and Catechol.

31-117;

## **1928:** ortho-**METHYL**-para-tertiary-**BUTYL CYCLOHEXANOL**



$C_{11}H_{22}O = 170.30$

Colorless crystalline mass or semi-liquid mass of crystals in a viscous liquid.

The commercial product is usually a mixture of the solid *trans*-isomer and the liquid *cis*-isomer. The former is the desirable odor.

Almost insoluble in water, soluble in alcohol and oils. Melts at approximately 45° C. to a viscous, colorless liquid.

*trans*-isomer: Powerful floral-woody and tenacious odor. The floral tones are not entirely sweet, but warm and pleasant.

*cis*-isomer: Camphoraceous-minty, powerful and tenacious odor. Somewhat sweet but the camphoraceous tone makes it seem rather dry.

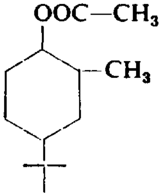
Perfumers generally prefer the *trans*-isomer for its ability to enhance floral notes, give lift and power, and support woody notes with little or no addition to camphoraceous notes.

This material, rarely offered under its proper chemical name, is used in perfume compositions varying from woody-musky to heavy sweet floral, and its powerful lift is utilized in soap perfumes, etc.

In spite of its apparent "unnatural" character, it can be used in concentrations up to 6 or 8% even in strictly floral compositions, and higher in woody-musky odor types.

Prod.: by hydrogenation of *para-tertiary*-Butyl-*ortho*-cresol.

## **1929:** ortho-**METHYL**-para-tertiary-**BUTYL CYCLOHEXANYL ACETATE**



$C_{13}H_{24}O_2 = 212.34$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, musty-fruity, somewhat floral odor with a dry-green undertone. Overall, not a very "natural" odor. Fair to good tenacity.

This ester has found a little use in perfume compositions, but it does not seem to have the ability to "lift" fragrances the same way as the parent alcohol has. The situation resembles that of Menthol and Menthyl acetate, the former having the powerful cooling effect, the latter being mild, almost nondescript and with little or no ability to "lift" a fragrance.

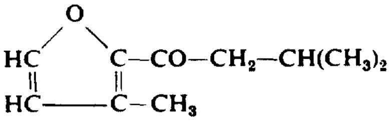
The author sees no strong future for this ester as a fragrance material.

Prod.: by direct esterification of the alcohol with Acetic anhydride or with Acetic acid under azeotropic conditions.

(See previous monograph).

## **1930:** 3-**METHYL**-iso-**BUTYL**-2-**FURYLKETONE**

*iso*-Butyl-*3*-methyl-*2*-furylketone.
*3*-Methyl-*2*-*iso*-valeroyl furan.
"Furylmethyl-*iso*-butylketone".
"Elsholtzia ketone".
Elsholtzione.



$C_{10}H_{14}O_2 = 166.22$

Pale yellowish mobile liquid. B.P. 210° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sharp minty, herbaceous, Rue-like odor of moderate to poor tenacity.

This material may not be used as such in perfumes or flavors, but the author believes that it has great possibilities at least in the further studies of related chemicals for flavor use. Its occurrence in certain plants in very large percentages of the volatile oils is interesting, and the plants themselves have had medicinal or food-additive value for ages.

The odor is not inviting to extensive perfumery experiments, and if the cost can not be brought down to level with commercial chemicals of similar odor type, it has no future as such in perfumery.

The close relationship of this ketone with those identified in Perilla oil certainly tempts to further investigation, and the fact that Methylfurans have application in flavors should encourage the perfume chemist or flavorist to search for new and useful derivatives in this chemical family.

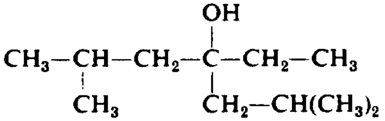
Prod.:

1) by isolation from the essential oil of Elsholtzia cristata in which the ketone occurs to the extent of 75 to 85%.
2) from *3*-Methylfuran to *3*-Methylfurfural via the oxime. Then to the cyanide and by Grignard reaction to subject ketone.

69-155; 90-777;

## 1931: 5-METHYL-3-iso-BUTYL-3-HEXANOL

*2,6*-Dimethyl-*4*-ethyl-*4*-heptanol.



$CH_3-CH(CH_3)-CH_2-C(OH)(CH_2-CH(CH_3)_2)-CH_2-CH_3$

$C_{11}H_{24}O = 172.31$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

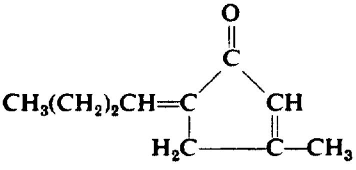
Sweet anisic-green, slightly earthy-spicy-fruity odor with pulegonic-minty emphasis and fair to good tenacity.

This alcohol, developed for entirely different industrial purposes, has been recommended for use in perfume compositions.

It gives interesting effects in Geranium, Lavender and Citrus colognes, particularly in the topnote compositions for colognes. Its very complex odor (considering that it is supposedly one single chemical!) blends excellently with light and medium light herbaceous-floral notes.

(Sample: Air Reduction Chemical Co., U.S.A.).

## 1932: 3-METHYL-5-n-BUTYLIDENE CYCLOPENTEN-2-ONE-1



$C_{10}H_{14}O = 150.22$

Pale yellowish oily liquid.

Very slightly soluble in water, somewhat soluble in hot water, soluble in alcohol and oils.

Warm-caramellic, fruity odor reminiscent of Strawberry.

Sweet fruity, "cooked" Strawberry flavor in dilutions below 20 ppm.

This ketone has been used and is still used to some extent in flavor compositions, rarely in perfumes.

It could be used as a modifier in fruity-floral bases, since it blends excellently with the Jasmone-derivatives and isomers, and also with the Ionones.

It plays only a minor part in the Strawberry flavor picture, but could be used in a variety of flavor types, Caramel, Rum, Raspberry, Vanilla, etc.

Prod.: from *3*-Methylcyclopentenone by condensation with *n*-Butyraldehyde.

(Heine & Co., patent).
4-334;

## 1933: METHYL-iso-BUTYLKETONE

*4*-Methyl-*2*-pentanone.
*iso*-Butylmethylketone.
*iso*-Propylacetone.
*iso*-Hexanone-*2*.

$CH_3—CO—CH_2—CH(CH_3)_2$

$C_6H_{12}O = 100.16$

Colorless liquid. Sp.Gr. 0.80. B.P. 117° C.

2% soluble in water, soluble in alcohol, miscible with oils. Soluble in Propylene glycol and Glycerin.

Powerful and diffusive ethereal-fruity odor of poor tenacity.

Sweet-fruity, ethereal flavor in dilutions below 20 ppm. At higher concentrations the flavor appears more pungent, chemical and sharp.

This ketone finds a little use in perfume compositions as a masking agent in industrial fragrances, etc.

It is more frequently used in flavor compositions for imitation Peach, Orange, Banana, Pineapple, Pear, Rum, etc. and in fruit complexes.

The normal concentration is about 5 to 8 ppm in the finished product.

Lately, it has found use in the reconstitution of flavor in Orange juice.

G.R.A.S. F.E.M.A. No.2731.

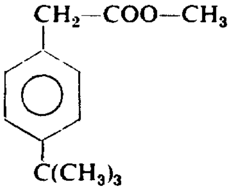
Prod.:

1) by oxidation of Methyl-*iso*-butylcarbinol. However, the latter is more often produced from the ketone which is a petrochemical, commercially available in volume.
2) from Mesityloxide by hydrogenation.

26-600; 31-80; 66-515; B-I-691; 160-1146; (see also: Journal of Food Science 29, 790, 1964).

## 1934: METHYL-para-tertiary-BUTYL PHENYLACETATE

*para-tertiary*-Butyl methylphenylacetate.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, somewhat woody-camphoraceous odor of good tenacity. The fruity topnote seems to be accompanied by a dry undertone which gives a very unusual and peculiar combination odor.

This ester is used in Chocolate, Cocoa, Honey and various fruit flavor compositions for its power and specific, "roasted" chocolate-like effect.

The normal use concentration is about 0.5 to 2 ppm in the finished product.

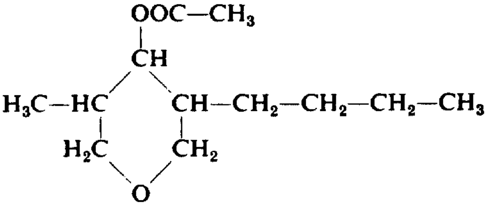
It is interesting to note that this ester is an empirical isomer of Amyl phenylacetate, which is also a chocolate-flavor chemical.

G.R.A.S. F.E.M.A. No.2690.

Prod.: by direct esterification of *para-tertiary*-Butyl phenylacetic acid with Methanol.

## 1935: 5-METHYL-3-BUTYL-TETRAHYDROPYRAN-4-YL ACETATE

Main component of
"Tepyl acetate" (U.O.P. Chem. Co.).
- and many other specialties.



$C_{12}H_{22}O_3 = 214.31$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm, oily-herbaceous floral and sweet-earthy odor resembling certain notes of the Jasmin fragrance picture. Moderate tenacity and excellent stability.

This material, known for many years, but only slowly becoming a standard item on the perfumer's shelf, was recommended for soap perfumes and perhaps therefore not often considered by the perfumer for other purposes. It is now widely used as component of artificial Jasmin and other floral bases, Tuberose, Gardenia, etc. and its effect in Lavender has been established by successful compositions. It blends exceptionally well with Amylcinnamic aldehyde, Benzyl- and Linalylesters, Opopanax and Oakmoss, Amylsalicylate, etc. and it has a pleasant mellowing effect on hay-like or herbaceous notes, including Labdanum.

The perfume chemicals market abounds in Jasmin materials, but very few of these are the "large volume" components, or more than trace components. The title material can be used in relatively high concentration in Jasmin base, while in general, 2 to 4% will introduce mellowing herbal tones.

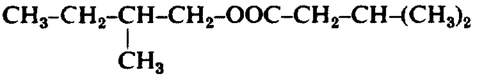
As a minor component in a great number of "chemicals", sold under trade names (see monograph: Nonanediol-*1:3*-diacetate), the title Pyranylester has become very popular and new uses are suggested, while new combinations of the Pyranylesters, ethers, and the Nonane- and Decane-diol esters, etc. are developed, often by simple changes in the selection of fractions from the distillation of the reaction mixture (see above monograph).

The title ester is, however, quite unique and versatile, and it is most conceivable that other chemicals of related structure may prove very useful to the perfumer.

See also monograph: Tetrahydro pyranyl crotonate.

## 1936: 2-METHYLBUTYL-iso-VALERATE

*d-secondary*-Butylcarbinyl-*iso*-pentanoate.



$$CH_3\text{-}CH_2\text{-}\underset{\displaystyle CH_3}{\underset{|}{CH}}\text{-}CH_2\text{-}OOC\text{-}CH_2\text{-}CH\text{-}(CH_3)_2$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Herbaceous-fruity, slightly earthy odor of moderate tenacity.

Sweet-fruity, powerful, balsamic-herbaceous taste in dilutions below 50 ppm.

This ester is used in flavor compositions, mainly in artificial essential oils, e. g. Peppermint. It does not supply any "minty" effect, but it adds the sweet-balsamic, herbaceous note which is characteristic of the non-mentholic portion of Peppermint oil, a virtue for which Peppermint oil is often specifically valued.

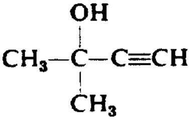
G.R.A.S. (1967 amendment).

Prod.: by direct esterification of *2*-Methylbutanol with *iso*-Valeric acid under azeotropic conditions.

(Sample: The Glidden Co.).

## 1937: 2-METHYL BUTYNOL

*2*-Methyl-*3*-butyn-*2*-ol.
The structure for this chemical has repeatedly been quoted erroneously in perfumery literature.



$$CH_3-\overset{\overset{\displaystyle OH}{|}}{\underset{\underset{\displaystyle CH_3}{|}}{C}}-C\equiv CH$$

$C_5H_8O = 84.12$

Colorless mobile liquid. B.P. 104° C. Sp.Gr. 0.86.

Solidifies in the cold, melts again at +3° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, green-ethereal, gassy odor, unpleasantly choking when undiluted, but quite pleasant, fresh-green when diluted.

The title alcohol was not originally intended to be a perfume chemical, but served as an intermediate in the "Hoffmann-laRoche-process" of making Methylheptenone (and further on to Linalool, etc.).

It also yields a Pentenol of some perfumery interest upon hydrogenation.

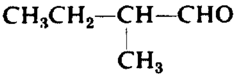
The subject alcohol has found some use in perfume compositions as a means of introducing "lift" and radiant power to certain types of fragrance, e. g. Hyacinth, Geranium, Lavender, etc. and particularly in soap perfumes, where this alcohol is quite stable.

Prod.: from Acetone and Acetylene in liquid Ammonia with Sodamide (or in Cellosolve with Potassium hydroxide). The process yields Methylbutynol which can be hydrogenated to Methylbutenol. This alcohol is treated with Diketene to produce Methylheptenone. Ethylation of this ketone yields Dehydrolinalool, the key material in making the "Roche" type Linalylesters.

66-318;

## 1938: alpha-METHYL BUTYRALDEHYDE

*2*-Methylbutanal-*1*.
Methyl ethyl acetaldehyde.



$$CH_3CH_2-\underset{\underset{\displaystyle CH_3}{|}}{CH}-CHO$$

$C_5H_{10}O = 86.14$

Note: Do not confuse with *3*-Methylbutanal-*1*, which is also called *2*-Methyl-*n*-butyraldehyde. That material is listed in the present work under: *iso*-Valeric aldehyde.

Colorless liquid. B.P. 93° C. Sp.Gr. 0.80.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful, choking odor when undiluted, but in extreme dilution the odor becomes tolerable, almost pleasant fruity-"fermented" with a peculiar note resembling that of roasted Cocoa or Coffee.

The taste is sweet, slightly fruity-chocolate-like in dilutions below 20 ppm. Pungent at higher concentrations.

This aldehyde is used in flavor compositions as a special topnote ingredient for certain fruit notes, Cocoa, Chocolate, etc. It gives part of the "overripe" or "fermented" note to an Apple flavor that may change the Apple flavor to a winey-Champagne-like flavor, a type which is commonly used in Gelatin candies.

The aldehyde is occasionally used in the reconstruction of certain essential oils.

G.R.A.S. F.E.M.A. No.2691.

Prod.:

1) e.g. by oxidation of active Amylalcohol (*secondary*-Butylcarbinol) isolated from fermentation Fusel oil.
2) The *racemic*- or *dl*-form is prepared from *secondary*-Butylmagnesium bromide plus Formaldehyde.
3) by reduction of Methylethylacetic acid.

66-477; B-I-682;

## 1939: METHYL BUTYRATE

Methyl-*n*-butanoate.

$CH_3\text{—}OOC(CH_2)_2CH_3$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. B.P. 103° C.
Sp.Gr. 0.90.

1.6% soluble in water, miscible with alcohol, Propylene glycol and oils.

Very diffusive and penetrating, sweet-ethereal, fruity odor. In extreme dilution reminiscent of Apple peel with a slightly fatty Peach-like undertone.

Sweet, but not very powerful taste in aqueous media. Apple-like or Banana-Pineapple-like in dilutions below 100 ppm.

This ester is occasionally used as a masking agent in industrial perfumes especially where the problem is to mask very volatile malodors, etc. The type of odor is particularly suitable to cover sulfuraceous odors.

It is, however, much more widely used in flavor compositions for imitation Apple, Banana, Pineapple, Melon, Peach, Rum and Arak, and in various fruit complexes.

The concentration used is equivalent to about 20 to 100 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2693.

Prod.: by direct esterification of Methanol with *n*-Butyric acid preferably under azeotropic conditions.

4-88; 33-732; 77-185; 86-90; 103-80; 160-892; 66-586;

## 1940: METHYL-iso-BUTYRATE

Methyl-*2*-methylpropanoate.
Methyl dimethylacetate.

$CH_3\text{—}OOC\text{—}CH(CH_3)_2$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. B.P. 93° C.
Sp.Gr. 0.89.

Slightly soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Milder and sweeter odor as compared to the *n*-butyrate, less Apple-like, more Apricot-like.

The flavor follows the odor in that it is less Apple-like, more sweet-Apricot or Peach-like (than the *n*-butyrate).

This ester finds use in flavor compositions, mainly in fruit flavors including the popular "Tutti-frutti" or "Juicy-fruit" complexes, to which the ester adds a powerful and diffusive initial note.

The concentration used is normally about 20 to 200 ppm in the finished product.

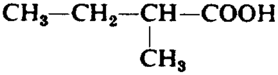
G.R.A.S. F.E.M.A. No.2694.

Prod.: by direct esterification of Methanol with *iso*-Butyric acid under azeotropic conditions.

66-586; 86-94; 90-196; 103-80; 160-1058;

## 1941: alpha-METHYL BUTYRIC ACID

Butane-*2*-carboxylic acid.
*2*-Methylbutanoic acid.
Methylethyl acetic acid.
Ethyl methyl acetic acid.
*optically active iso*-Valeric acid.
Exists in *dextro*-form (natural), *laevo*-form and *dl*-form (synthetic).



$$CH_3\text{—}CH_2\text{—}\underset{\displaystyle CH_3}{\underset{|}{CH}}\text{—}COOH$$

$C_5H_{10}O_2 = 102.14$

Colorless liquid. Sp.Gr. 0.94. B.P. 177° C.

Slightly soluble in water, soluble in alcohol and oils. Also soluble in Propylene glycol, poorly soluble in Glycerin.

Pungent, acrid odor reminiscent of Roquefort cheese and other cheeses, but not quite as repulsive and stinging as the odor of *n*-Valeric acid or *iso*-Valeric acid.

Acrid-acid taste, which becomes quite pleasant and fruity-sour at dilutions below 10 ppm.

This acid finds limited use in perfume compositions, mostly in artificial essential oils.

It is also used in flavor compositions for its contribution to Cheese flavor, Butter imitation, cream, Chocolate, etc.

The concentration is normally mere traces, equivalent to 0.5 to 5 ppm in the finished product.

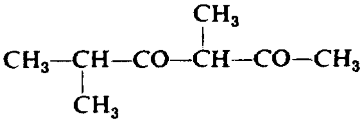
Prod.: by oxidation of fermentation (Fusel)-Amyl alcohol. The acid can also be manufactured synthetically.

G.R.A.S. F.E.M.A. No.2695.

66-571; 90-78; 160-894;

## 1942: METHYL-iso-BUTYRYL ACETONE

*3,5*-Dimethyl-*2,4*-hexane dione.



$$CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CO-\overset{\displaystyle CH_3}{\overset{|}{CH}}-CO-CH_3$$

$C_8H_{14}O_2 = 142.20$

Colorless mobile liquid. B.P. 177° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Pleasant, fruity, slightly creamy odor with vague resemblance to Banana.

Sweet, fruity-creamy, slightly caramellic taste.

This diketone has been suggested for use in flavor compositions, but is not specifically mentioned in the U.S.A. Federal Register as a G.R.A.S. material.

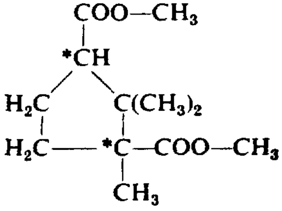
It could, however, find use in imitation Butter, Cream, Banana, Mango, Peach, etc., particularly for flavoring of dairy products or chocolate candy.

Prod.: by condensation of Ethylacetate and Ethyl-*iso*-propylketone.
31-82;

see also: Journal of American Chemical Society 1944, 66, 1220 and same Journal: 1945, 67, 284 and 1510.

## 1943: METHYL-iso-CAMPHOLATE

Dimethyl-*trans*-campholate.
*trans*-Campholic acid, Dimethylester.
The material exists in *d*- and *l*-form.



$C_{12}H_{20}O_4 = 228.29$

*) Asymmetric C-atom.

White crystalline material. M.P. 70° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar, sweet-and-dry, fruity-woody odor of good tenacity.

Concentrations near 20 ppm have a Banana-like taste, but it is accompanied by a slight bitterness.

This ester has been suggested for use in flavor compositions for its Banana-like effect. However, the author finds that this material has very little effect at the level of concentration where its flavor is absolutely agreeable.

On the other hand, the ester gives very interesting effects in perfume compositions of Mimosa and Cassie-type. Well blended with lasting sweeteners such as Anisyl acetate, Heliotropyl acetone, etc. and with selected Ionones, Methylionones, etc. it can give very pleasant variations of the Mimosa theme.

3-289; B-IX-34;
see also: 1-669; 1-712;

## 1944: METHYL CAPRINATE

Methyl decanoate.
Methyl decylate.
Methyl caprate.

$CH_3$—OOC—$(CH_2)_8CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 228° C.
Solidifies in the cold, melts at minus 18° C.

Insoluble in water, soluble in alcohol and oils.

Oily-winey, slightly fruity odor when pure. Samples containing traces of Decanoic caid will have a perceptible and usually undesirable fatty undertone.

Winey-honey-like taste, quite powerful.

This ester finds a little use in perfume compositions such as Orris bases, woody fragrances and Mimosa bases. It blends excellently with the Ionones and the Cedarwood derivatives, Cyclohexane derivatives and alifatic aldehydes.

It is also used sparingly in certain flavor types, e. g. Brandy, Wine, Honey, Banana, Coconut, etc.

Prod.: by direct esterification of *n*-Decanoic acid with Methanol, preferably under azeotropic conditions.

26-602; 86-92; 90-212; 103-81; 160-900;
B-II-356;

## 1945: METHYL CAPROATE

Methyl hexoate.
Methyl hexanoate.
Methyl hexylate.

$CH_3$—OOC—$(CH_2)_4CH_3$

$C_7H_{14}O_2 = 130.19$

Colorless oilyl liquid. Sp.Gr. 0.89.
B.P. 151° C.

Insoluble in water, soluble in alcohol and oils.

Powerful ethereal and diffusive, sweet odor of Pineapple-Apricot type. Poor tenacity.

Sweet-fruity, not very powerful, Pineapple-Apple-Apricot type taste.

This ester is rarely used in perfumery, but it finds some application in flavor compositions, mainly in Strawberry and Pineapple flavor imitations. It may also enter in traces in an Apple flavor or the so-called "wine" flavor which is a variation of Apple-Champagne flavor.

The concentration used is normally as low as 4 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2708.

Prod.: by direct esterification of *n*-Caproic (*n*-Hexanoic) acid with Methanol, preferably under azeotropic conditions.

4-88; 26-602; 34-1230; 86-90; 90-199; 160-902;
B-II-323;

## 1946: METHYL-iso-CAPROATE

Methyl-*4*-methylvalerate.
Methyl-*iso*-butylacetate.
Methyl-*4*-methylpentanoate.

$(CH_3)_2CH(CH_2)_2COO$—$CH_3$

$C_7H_{14}O_2 = 130.19$

Colorless liquid. Sp.Gr. 0.89. B.P. 143° C.

Insoluble in water, soluble in alcohol and oils.

Sweet-fruity, Pineapple-like taste.

This ester finds a little use in flavor compositions, mainly as component of imitation Pineapple, sometimes Strawberry.

The concentration used is equivalent to about 10 to 50 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2721.

Prod.: by direct esterification of *4*-Methylpentanoic acid with Methanol preferably under azeotropic conditions.

90-200;

## 1947: METHYL CAPRYLATE

Methyl octanoate.
Methyl octylate.
Methyl octoate.

$CH_3{-}OOC(CH_2)_6CH_3$

$C_9H_{18}O_2 = 158.24$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 193° C.

Insoluble in water, soluble in alcohol and oils.

Powerful winey-fruity, Orange-like odor of moderate tenacity.

Oily-fruity, somewhat Orange-like taste.

This ester finds a little use in perfume compositions, mostly in Orris compositions, Oriental bases, Opopanax, etc.

It is used in flavor compositions as a fortifier in Pineapple imitation, in various berry flavors, and Citrus complexes.

The concentration used is normally about 0.20 up to 40 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2728.

Prod.: by direct esterification of *n*-Octanoic acid with Methanol e. g. under azeotropic conditions.

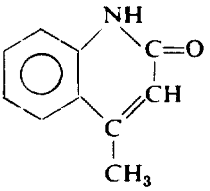
26-602; 35-404; 77-19; 86-90; 90-206; 160-902; B-II-348;

## 1948: METHYL CARBOSTYRIL

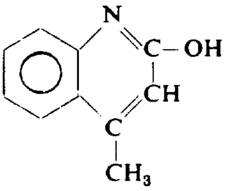
A number of isomers are covered by this name.

This monograph describes:
*4*-Methyl-*2*-hydroxyquinoline.
*4*-Methyl-*2*-quinolinol.
*2*-(*1*)-Lepidine.
*gamma*-Methyl-*2*-quinolinol.

This product exists in two forms:



4-Methyl-*alpha*-quinolone,
(so-called Lactam-form).



*2*-Hydroxy-*4*-methylquinoline,
(so-called Lactim-form).

$C_{10}H_9NO = 159.19$

Colorless needlelike crystals. M.P. 217° C.
B.P. higher than 350° C.

Slightly soluble in cold water, soluble in hot water and alcohol. Poorly soluble in most oils.

Pungent, sweet-aromatic odor, somewhat related to the prototype "Quinone"-type odor, but heavier, less buttery, more medicinal. Very tenacious and penetrating.

This material has been suggested for use in perfume compositions as trace component of certain floral bases, artificial flower absolutes and animal-floral fragrance types. It does impart very natural and powerful notes to Jasmin, Tuberose, Civet-complexes, etc. but there has been a great deal of reluctance in the common application of subject material, since it is not sufficiently investigated with respect to its tolerance on human skin, etc.

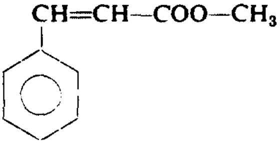
Prod.:

1) from Quinoline by hydroxylation, heating with Potassium hydroxide, followed by Methylation of the Hydroxyquinoline.
2) from *4*-Methylquinoline (= Lepidine) by heating with dry Potassium hydroxide.

26-602; 69-621; 69-590; 160-914; B-XXI-304;

## 1949: METHYL CINNAMATE

Methyl-*3*-phenylpropenoate.
Methyl cinnamylate.
The commercial material is the *trans*-isomer.



$C_{10}H_{10}O_2 = 162.19$

White or colorless crystalline mass.
M.P. 38° C. B.P. 263° C. Sp.Gr. 1.04 (liquid).

The *cis*-isomer (not a commercial material) is liquid.

Insoluble in water, soluble in alcohol, Propylene glycol, Mineral oil and oils.

The material may polymerize under certain storage conditions, the polymerization being enhanced e. g. by intermittent heating to melt the material in the storage container. Polymerization causes turbidity of the liquid material, or in severe cases gelatinization after which the material no longer melts to a clear liquid, and it loses odor, becomes practically insoluble in above solvents.

Powerful, yet very tenacious, fruity-balsamic odor, in extreme dilution more fruity, Strawberry-like, less balsamic.

Sweet and fruity, Cherry-Strawberry-like taste in dilutions below 20 ppm.

This ester is widely used in perfume compositions, but normally at very low concentration. It imparts power and sweet-fruity, balsamic "Oriental" notes to Ambre bases, Citrus colognes (where it blends excellently with Labdanum products), Carnation (where it introduces freshness), Narcisse, Lavender, Fruit and Spice blends, etc.

Its power and low cost makes it useful in soap and detergent perfumes and many types of household product fragrances.

It is used frequently in flavor compositions for imitation Butter, Cherry, Strawberry, Cream, Grape, Liqueurflavors, Mouthwash flavors, and in Peach, Plum, Vanilla, etc. in trace amounts.

The normal concentration is about 2 to 15 ppm, but it may be as high as 40 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.2698.

FCC-1964-857.

Prod.: by direct esterification of Cinnamic acid with Methanol, preferably using a low-heat process such as azeotropic esterification.

26-602; 4-89; 34-461; 67-996; 77-194; 86-90; 90-336; 100-674; 103-82; 106-242; 160-926; B-IX-581;

## 1950: alpha-METHYLCINNAMIC ALCOHOL

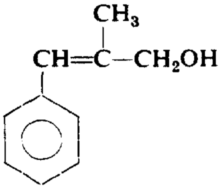
*alpha*-Methyl-*3*-phenyl-*2*-propen-*1*-ol.

NOTE: The perfumery literature and trade are particularly known for their confusing nomenclature, and this item is one which has suffered a great deal from such incorrect labelling. It has often been called *beta*-Methylcinnamic alcohol, and, unfortunately, a chemical with that name does exist.

This work does not claim to be faultless, but it aims at elucidating and possibly eliminating the most common cases of confusing nomenclature.

The material which was for many years sold under the name *beta*-Methylcinnamic alcohol was, indeed, the *alpha*.

More recently, the acetate of the *beta*-alcohol has become a commercially available perfume chemical.



$C_{10}H_{12}O = 148.21$

Colorless, slightly viscous liquid. Sp.Gr. 1.04.

Solidifies in the cold, melts again at 19° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, balsamic-floral, tenacious odor of "Oriental" type. It is less "Cinnamon-like", and more "Styrax-like" than Cinnamic alcohol, but it does not compete favourably with a pure Cinnamic alcohol with respect to natural floral notes.

This alcohol was introduced during a period of scarcity of Styrax, and was particularly promoted as a basis for making artificial Styrax. It has also the convenience (which seems to be of psychological power) of being liquid. Many perfumers have a subconscious inhibition when it comes to using a solid material, melting or dissolving it, when a liquid material of similar effect is at hand.

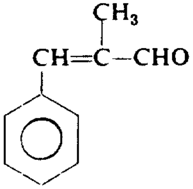
However, this alcohol did not seem to fill in all the many uses of Styrax, and could not economically compete with Cinnamic alcohol. It still finds some use as a modifier in balsamic and Oriental blends, but natural Styrax has again become freely available at a very attractive price.

Prod.: by regulated hydrogenation of *alpha*-Methylcinnamic aldehyde.

156-85;
(original sample from Trubek Laboratories, 1958).
(Later samples from several other sources).

## 1951: alpha-METHYL CINNAMIC ALDEHYDE

*alpha*-Methylcinnamal (see note below).
*2*-Methyl-*3*-phenyl-*2*-propenal.



$C_{10}H_{10}O = 146.19$

Yellowish oily liquid. Sp.Gr. 1.04.

Insoluble in water, Mineral oil and Glycerin. Soluble in alcohol and oils.

Powerful, sweet-herbaceous, but primarily Cinnamon-spicy, warm odor of moderate tenacity. Sweeter and less pungent than Cinnamic aldehyde, more haylike and floral than that aldehyde.

This material finds some use in perfume compositions, where its superior stability makes it a modifier for Cinnamic aldehyde, sometimes even a substitute for that. It adds warm-spicy notes and a trace of floral character, it blends well with Cinnamic alcohol, with woody or Clove-spicy notes, heavy floral notes including certain types of Rose, etc. It gives interesting effects of great power with Petitgrain (Cashmere-type odor), and it shows less tendency of discoloration in soap than the Cinnamic aldehyde.

It is also used in flavor compositions, mainly for spice blends, and for certain fruit complexes. Spicy chewing gum, and spicy mouthwash have had a comeback, and this aldehyde is frequently used where the spiciness with less "bite" is desirable.

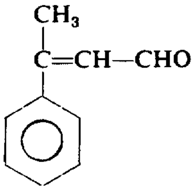
The concentration in finished products is about 0.5 to 30 ppm, except in chewing gum where it usually reaches 250 to 450 ppm.

G.R.A.S. F.E.M.A. No.2697.

FCC-1964-859.

Prod.: by condensation of Propionic aldehyde with Benzaldehyde under alkaline conditions.

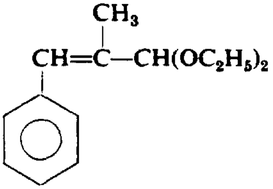
4-97; 68-986; 93-148; 156-91;
NOTE: True *beta*-Methylcinnamic aldehyde has the structure:



*3*-Methyl-*3*-phenyl-*2*-propen-*1*-al.

It is not considered as a perfume material but it is mentioned here for the sake of clarification of the common confusion and erratic use of the name "*beta*-Methylcinnamic-" instead of the correct "*alpha*-Methylcinnamic-".

## **1952:** alpha-**METHYLCINNAMIC ALDEHYDE DIETHYLACETAL**



$C_{14}H_{20}O_2 = 220.31$

Pale yellowish oily liquid, or almost colorless liquid. Sp.Gr. 0.97. B.P. 255° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Pleasant, sweet-oily, green and very faintly spicy-herbaceous odor of good tenacity.

This acetal has been suggested for use in perfume compositions where a hazard of oxidation of the parent aldehyde may be present and the overall conditions are not acid.

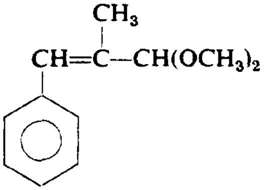
However, the acetal is not a mild substitute for the aldehyde, it has a distinctly different odor, less spicy, more green and herbaceous, much weaker.

It could find some use in heavy floral or Oriental bases, etc.

Prod.: from *alpha*-Methylcinnamic aldehyde plus Ethylformate and sulfuric acid.

93-148;

## **1953:** alpha-**METHYLCINNAMIC ALDEHYDE DIMETHYLACETAL**



$C_{12}H_{16}O_2 = 192.26$

Pale yellowish or almost colorless oily liquid. An absolutely aldehyde-free material is colorless. Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils.

Mild, warm, oily-herbaceous, slightly green-woody odor.

This material was developed in search of new and interesting Acetal-odors, but since the parent aldehyde is comparatively stable, the Acetal does not have this specific advantage over its parent aldehyde and much of the interest in the Acetal is lost if it does not at least have a very unusual odor or fragrance effect.

Briefly, a material of practically no interest to the perfumer or flavorist.

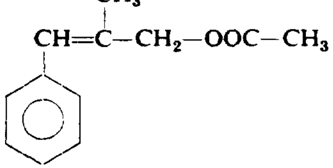
Prod.: by condensation of *alpha*-Methylcinnamic aldehyde and Methanol, e. g. by dry Hydrochloric gas treatment in the cold.

93-148;

## **1954:** alpha-**METHYL CINNAMYL ACETATE**

*2*-Methyl-*3*-phenyl-*2*-propen-*1*-yl acetate.

NOTE: The perfumery literature often refers to: *beta*-Methyl cinnamyl acetate (true material – see below), when the correct name should be *alpha*-Methyl cinnamylacetate.



$C_{12}H_{14}O_2 = 190.24$

Colorless liquid.

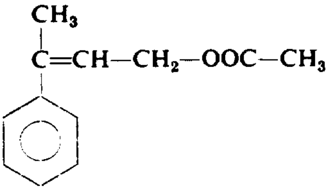
Almost insoluble in water, soluble in alcohol and oils.

Sweet and slightly spicy, warm, yet refreshing odor with distinctly fruity notes, in dilution appearing Strawberry-like. Good tenacity.

This acetate, like its parent alcohol, is often called *beta*-Methylcinnamyl acetate, but modern chemists (including the British Chemical Society) encourage the use of the name *alpha*-Methyl- for these chemicals. The ester finds some use in perfume compositions, mainly of the Oriental and pungent-floral-fruity type. It blends very well with Amylsalicylate, Patchouli oil, Styrax and Labdanum, the Ionones, etc. and gives new effects with Ethyl methyl phenyl glycidate in lipstick fragrances.

Prod.: by acetylation of *alpha*-Methylcinnamic alcohol (see monograph).

NOTE: True *beta*-Methyl cinnamyl acetate has the structure:



$C_{12}H_{14}O_2 = 190.24$

The material does exist, but the author believes that it has no application in perfumes or flavors.

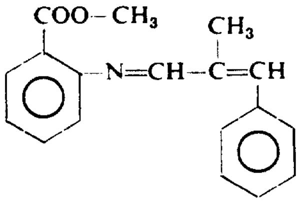
Prod.: e. g. by condensation of Ethylacetate with Ethylbenzene.

The confusion in the use of above names is mainly due to the fact that Cinnamic alcohol has been called "*gamma*"-Phenylallyl alcohol, thus creating the name "*beta*"- for the Methyl-substitution in the neighbour Carbon atom.

## **1955:** alpha-**METHYLCINNAMYLIDENE METHYLANTHRANILATE**

Methyl-*N*-*alpha*-methylcinnamylidene anthranilate.

A Schiff's base.



$C_{18}H_{17}NO_2 = 279.34$

Intensely yellow oily liquid.

Practically insoluble in water, soluble in alcohol and oils. Very slightly soluble in Propylene glycol.

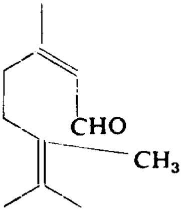
While the Schiff's base from Cinnamic aldehyde is dark and unattractive, and possesses a rather uninteresting odor, the base prepared with *alpha*-Methylcinnamic aldehyde is only intensely yellow and has a powerful, deep-sweet, floral-balsamic odor of interesting possibilities.

The base is used in perfume compositions to lend depth and warm-powdery undertones in heavy florals, even in certain types of Rose. It has good tenacity and blends well with Hydroxycitronellal, the "rose alcohols", the floral Lactones, Petitgrain oil, Cinnamic alcohol and its esters, etc.

Prod.: by condensation of Methylanthranilate with *alpha*-Methylcinnamic aldehyde at moderate temperature and under continuous removal of condensation water.

## 1956: 3-METHYL CITRAL

*3,6,7*-Trimethyl-*2,6*-octadienal.
The commercial product is normally a mixture of
*cis*- and *trans*-isomers with smaller amounts of other isomers.
Sometimes called: Methyl-*3*-citral.



$C_{11}H_{18}O = 166.27$

Colorless liquid. Sp.Gr. 0.90. B.P. 228° C. (slightly higher for the *trans*-isomer, slightly lower for the *cis*-isomer).

Almost insoluble in water, soluble in alcohol and oils.

Sweet and refreshing Lemon-like fruity odor of moderate tenacity. Not nearly as "lemony" as Citral, but sweeter: Does not have the initial "punch" often observed in commercial grade Citral, and the Methylcitral is more tenacious. Overall less versatile than Citral.

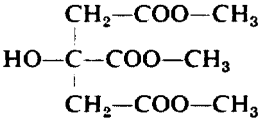
This aldehyde has been suggested for use in perfume compositions as a modifier for Citral, or as a refreshing note without typical Lemon note. However, the cost of the title material is absolutely prohibitive for its use in general perfume creation at the concentrations normally needed to obtain a desirable effect.

Prod.: (several methods) e. g. by oxidation of *3*-Methyl-Linalool, or: from Citral and Dimethylsulfate plus Pyridine by heating in Diethylene glycol.

4-89; 86-90; 89-102; 163-49; 163-220;

## 1957: METHYL CITRATE

Trimethyl citrate.



$$\begin{array}{l} \quad\ \ CH_2{-}COO{-}CH_3 \\ \quad\ \ \ \ | \\ HO{-}C{-}COO{-}CH_3 \\ \quad\ \ \ \ | \\ \quad\ \ CH_2{-}COO{-}CH_3 \end{array}$$

$C_9H_{14}O_7 = 234.21$

Colorless crystals. M.P. 79° C.
B.P. 287° C. (decomposes).

Slightly soluble in water, soluble in alcohol and oils.

Virtually odorless when pure, the commercial material has a faint, ethereal-fruity, bland odor.

Slightly bitter taste in high concentration, practically tasteless below 20 ppm.

This material has been suggested for use in perfume formulations as a fixative and blender in various powerful floral bases, etc. The ethylester is more commonly used for this purpose, partly because it has a slightly sweeter odor, partly because it is more stable.

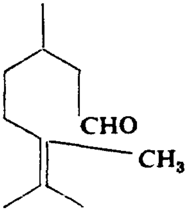
The author knows of no significant use of this ester in flavor compositions, other than that of a "diluent" or "blender".

Prod.: by direct esterification of Citric acid with Methanol using the old-fashioned method with 3% sulfuric acid and reflux to complete the esterification.

26-208; 66-1190; 160-928; B-III-567;

## 1958: 3-METHYLCITRONELLAL

*3,6,7*-Trimethyl-*6*-octenal.
*3*-Methyl-*beta*-citronellal.
(The *alpha*-isomer is also known).



$C_{11}H_{20}O = 168.28$

Colorless liquid. Sp.Gr. 0.86. B.P. 226° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils, but not in Glycerin.

Sharp, but not harsh, Lemon-like and slightly green odor. Sweeter and less harsh than Citronellal, also less diffusive. Fair to moderate tenacity.

Lemon-like, but not sweet flavor in concentrations near 10 ppm.

This aldehyde has been suggested for use in perfume compositions as a modifier or substitute for Citronellal, which is not only very unstable, but also has an unpleasant, pungent-harsh, penetrating odor, difficult to utilize in household product fragrances.

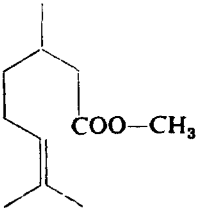
However, the title aldehyde is still too expensive to be able to compete with Citronellal-type materials (including Citronella oil), since its synthesis involves the use of more costly starting materials.

Prod.:

1) from *3*-Methyl linalool via *3*-Methylcitral by hydrogenation to the title material.
2) from Citral via *3*-Methylcitral to the title material.

89-67; 163-220; 163-358;

## 1959: METHYL CITRONELLATE



$C_{11}H_{20}O_2 = 184.28$

Colorless mobile liquid. Sp.Gr. 0.91.
B.P. 216° C.

Almost insoluble in water, soluble in alcohol and oils.

Refreshing, winey-green, fruity and Brandy-like, Apple-like odor of moderate to poor tenacity.

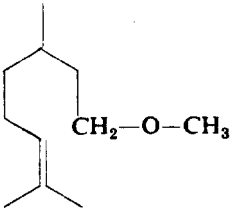
This ester, not often offered commercially, has found a little use in perfume compositions, mainly as part of new topnote complexes with natural-green materials for Rose, Muguet, Peony, and in refreshing, "outdoor"-type fragrances, etc.

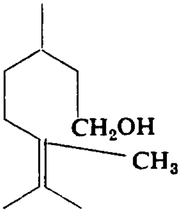
Prod.: by oxidation of Citronellol (or Citronellal) with $Cr_2O_3$ to yield Citronellic acid, which is esterified with Methanol.

86-91; 90-133; 90-240;

## 1960: METHYLCITRONELLOL

This monograph describes:
*3,6,7*-Trimethyl-*6*-octenol ("true" *3*-Methylcitronellol)
but the author believes that the name is often confused with the name for Citronellol methylether, or with Ethyl citronellol, which is the next higher homologue of Citronellol.


Citronellol methylether.
(See also monograph for
Ethyl Citronellol).


Methyl citronellol (title material).
*3,6,7*-Trimethyl-*6*-octenol.

$C_{11}H_{22}O = 170.30$

Colorless liquid. Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet-rosy, moderately tenacious odor. Less minty, but also less fresh-diffusive when compared to Citronellol, overall lighter, milder, more lasting.

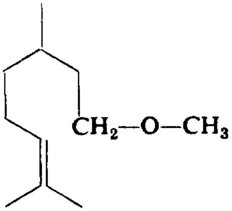
This alcohol has been suggested for use in perfume compositions as a modifier for Citronellol in Rose bases, etc. However, at a much higher cost and with no unusual or very highly desirable effect, this alcohol has little chance among the conventional "Rose alcohols" in creative perfumery.

Prod. (title material): from *3*-Methylcitral via Methylcitronellal. (Citronellyl methylether): from Citronellol with Dimethylsulfate and Pyridine by heating in Diethylene glycol.

7-124; 4-89; 163-49;

## 1961: METHYL CITRONELLYL ETHER

Citronellyl methylether.
(Not to be confused with Methyl citronellol).


$C_{11}H_{22}O = 170.30$

Colorless liquid.
Insoluble in water, soluble in alcohol and oils.

Fresh-rosy, green-leafy type of odor with a "wet vegetable" note of attractive naturalness. Moderate to poor tenacity.

This ether has been suggested for use in perfume compositions, but it is rarely offered commercially, although many ethers of Citronellol, Geraniol, Linalol and related alcohols have been prepared in search of new floral-green materials. Quite a large number of these ethers have very interesting and attractive odors, and it is rather surprising that very few are offered commercially.

The title ether could find use in modern fragrances, particularly as part of novel top-note complexes with Citrus, Galbanum or fresh-herbaceous materials, fruity notes, etc.

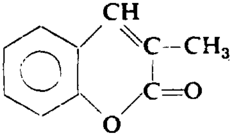
It blends very well with Bergamot, Estragon, Basil, Verbena and other distinguished top-note materials, and it is tolerated in the perfume composition at quite surprising concentrations. In other words, its pleasant level of application has a very considerable "range" from less than one percent up to 10 or 15%, in exceptional cases even higher than that.

Prod.: from Citronellol and Methanol by dehydration.

See also: 1960.
4-34;

## 1962: 3-METHYLCOUMARIN

*alpha*-Methylcoumarin.



$C_{10}H_8O_2 = 160.17$

Colorless needlelike crystals. M.P. 91° C. Almost insoluble in water, slightly soluble in cold alcohol, somewhat soluble in hot alcohol, soluble in most oils.

Powerful and rich, Tonka-like, sweet-herbaceous odor, somewhat drier than that of Coumarin. Good tenacity.

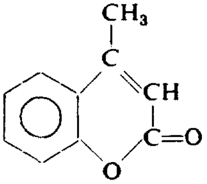
This Methylcoumarin finds some use in perfumery as a modifier for Coumarin and *6*-Methylcoumarin in Chypres, Oriental bases, Lavender compositions or Tonka-bases, etc. It blends extremely pleasantly with Oakmoss products and Bergamot for Chypre bases, and gives warm natural background to Lavender and other herbaceous fragrances.

Prod.: from Salicylaldehyde plus Propionic aldehyde (the conditions determine the yield of the *alpha*-isomer).

4-89; 31-166; 69-877; 86-91; 160-934; 103-303;

## 1963: 4-METHYLCOUMARIN

*beta*-Methylcoumarin.



$C_{10}H_8O_2 = 160.17$

Colorless needlelike crystals. M.P. 82° C.

Almost insoluble in water, slightly soluble in cold alcohol, soluble in hot alcohol and in most oils.

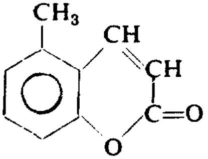
Dry, hay-like, rather weak Coumarin-type odor of good tenacity. Some observers claim that this isomer is odorless (69-877).

In any event, it is apparent that this particular isomer has failed to catch the interest of the perfumer. It is mentioned mainly for the sake of completing the picture of the Methylcoumarins.

Prod.: from *meta*-Cresol and Malic acid.

4-89; 5-212; 31-167; 69-877; 86-91; 160-934; B-XVII-336; 26-602; 103-303;

## 1964: 5-METHYLCOUMARIN



$C_{10}H_8O_2 = 160.17$

Colorless crystals. M.P. 66° C.

Practically insoluble in water, poorly soluble in alcohol, soluble in most oils.

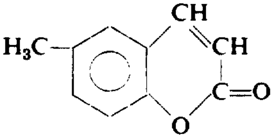
Sweet, rather musty, herbaceous-woody, tenacious odor. This isomer is, to the author's knowledge, not used in perfumery, although it has, from time to time, been offered by manufacturers of fine perfumery chemicals.

It is listed here for the sake of completing the monographs on the various commercially available Methylcoumarins.

69-877; 86-91; 103-303;

## 1965: 6-METHYLCOUMARIN

Toncarine. (Tonkarin).
Toncair.
6-Methyl benzopyrone.
Cocodescol.
Pralina.



$C_{10}H_8O_2 = 160.17$

Colorless or white needle-like crystals.
M.P. 75° C. B.P. 305° C.

Very slightly soluble in hot water, almost insoluble in cold water. Poorly soluble in cold alcohol, better in hot alcohol. Soluble in most perfume oils at concentration needed.

Semi-dry, herbaceous Tonka-like, but rather weak odor, more delicate than Coumarin, and more Fig- or Date-like in its fruity deep sweetness.

The taste is almost bitter at concentrations above 50 ppm, but turns sweet Vanilla-Tonka-like at lower concentrations.

This material is one of the most frequently used Methylcoumarins in perfumery, but its application is still much more limited than that of Coumarin. As a modifier in Chypres, Fougères, Lavender complex and many other types of Men's fragrance, it gives often a more pleasant terminal note that Coumarin itself.

This material is permitted in flavor compositions and its unusual stability towards heat and light (also appreciated in soap perfumes) makes it excellent for flavors in baked goods, etc.

It forms part of many imitation Butter, Caramel, Coconut, Date, Fig, Rootbeer and Vanilla flavors, fruit complexes, Nut compositions, etc.

The concentration in the finished product is normally about 1 to 40 ppm, lowest in presence of Vanillin which greatly enhances the flavor of Methylcoumarin (or vice-versa).

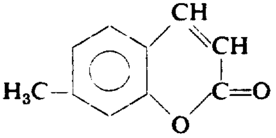
G.R.A.S. F.E.M.A. No.2699.

Prod.:

1) by condensation of *para*-Cresoldisulfonic acid with Fumaric acid under heat in presence of sulfuric acid.
2) by condensation of *para*-Homosalicylic aldehyde with Malonic acid in presence of Anilin, followed by heating to rearrange the Methylcoumarin carboxylic acid to the Lactone.
3) from Salicylic aldehyde with Propionic anhydride and Sodium propionate.

4-89; 5-216; 61-70; 69-877; 77-196; 86-91; 95-193; 96-180; 103-303; 106-244;

## 1966: 7-METHYLCOUMARIN



$C_{10}H_8O_2 = 160.17$

White crystals or microcrystalline powder.
M.P. 128° C.

Almost insoluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and in most oils.

Musty, slightly animal and leathery, tenacious odor with sweet-herbaceous undertones. The animal notes are very discrete, remotely resembling those of Costus, being more woody than herbaceous.

This material is very rarely offered commercially under its proper name, and the difficulties in manufacturing a reasonably pure quality add to the rather confusing odor descriptions occasionally published, leaving an impression that the various authors are not talking about the same chemical.

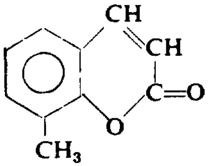
This Coumarin is used in perfume compositions where emphasis is upon the discrete leathery notes with refined Labdanum products, Oakmoss, Vetiver, etc. It performs excellently in modern versions of Men's fragrances with slightly woody or leathery-mossy notes under a rich, citrusy topnote. It is also used in women's perfumes often in combination with moderately Oriental notes and mostly in non-floral types.

Prod.:

1) from *meta*-Cresol plus Malic acid with concentrated sulfuric acid and heat.
2) by heating 7-Methylcoumarin carboxylic acid.

4-89; 37-726; 69-877; 95-193; 103-303;

## 1967: 8-METHYLCOUMARIN



$C_{10}H_8O_2 = 160.17$

White needlelike crystals. M.P. 110° C.

Almost insoluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and oils.

Very weak, semi-sweet, woody-herbaceous odor of considerable tenacity.

In view of the weakness of odor and lack of character in this Coumarin, it is reasonably safe to say that it has no important mission in perfumery and it is probably very rarely used at all.

It is listed in this work for the sake of completing the olfactory picture of the Methylcoumarins.

69-877;

## 1968: METHYL CROTONATE

Methyl-*alpha*-crotonate.
Methyl-*trans*-2-butenoate.

$CH_3—OOC—CH{=}CH—CH_3$

$C_5H_8O_2 = 100.12$

Colorless mobile liquid. B.P. 121° C.
Sp.Gr. 0.98.

Practically insoluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Powerful and diffusive, sharp and green-fruity odor of poor tenacity.

Concentrations below 50 ppm have a sweet, fruity, yet slightly pungent taste.

This ester has found a little use in perfumery, mostly as part of various fruit notes, Strawberry in particular. Indirectly, it may find its way into a multitude of fragrance types where such topnotes are applicable: Rose, Jasmin, Gardenia, Freesia, etc.

It performs very well with Clary Sage and Lavender, to which it gives power and lift, bringing these fragrances right up into the topnote section of the perfume.

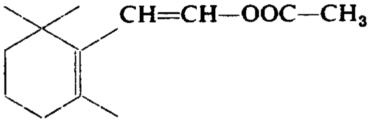
The Ethylester has been identified in the volatile oil from Strawberries.

Prod.: by direct esterification of Methanol with 2-Butenoic acid under azeotropic conditions.

26-602; 66-633; B-II-410;

## 1969: METHYL CYCLOCITRYLIDENE ACETATE

"Resedone". (This name is also used for the Ethyl-ester, see that monograph).



$C_{13}H_{20}O_2 = 208.30$

Colorless oily liquid.

Refreshing, vegetable-green, slightly earthy odor of moderate to poor tenacity. The odor has quite some resemblance to that of Linalyl methyl ether and related ethers, except that the subject ester has distinctly earthy notes.

This ester could find some use in perfume compositions as part of sophisticated topnote bases in aldehydic fragrance types, or in delicate florals, variations of Rose, etc. (Rose blends excellently with Reseda in Nature as well as in perfumery).

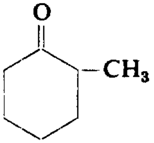
Although well known under specialty name for many years, this ester does not seem to have achieved much popularity, and it is practically non-existing in the average perfume laboratory.

Prod.: Cyclocitrylidene methanol by Acetylation.

5-354; 3-34; 3-109; 31-125; 4-38;

## 1970: 2-METHYL CYCLOHEXANONE

*ortho*-Methyl cyclohexanone.



$C_7H_{12}O = 112.17$

Colorless liquid. Sp.Gr. 0.93. B.P. 166° C.

Insoluble in water, soluble in alcohol and oils.

Somewhat harsh, minty-almondy, rather chemical odor. Poor tenacity. Slightly bitter-minty taste of considerable power.

This ketone has been suggested for use in soap perfumes, industrial fragrances, masking odors, etc. where its power and stability come to use. It may give "lift" to woody soap perfumes and add power to spicy-herbaceous fragrances, but its proper odor is not exactly beautiful.

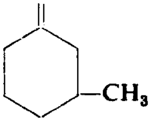
Prod.:

1) by methylation of Cyclohexanone,
2) by oxidation of *2*-Methylcyclohexan-*1*-ol.
3) from Cyclohexane with Carbon monoxide and Aluminum chloride in a Friedel-Craft's type reaction.

26-602; 31-87; 67-193; 67-198; 86-91; B-VII-14;

## 1971: 3-METHYL CYCLOHEXANONE

*meta*-Methyl cyclohexanone.



$C_7H_{12}O = 112.17$

Colorless liquid. Sp.Gr. 0.92. B.P. 169° C.

Insoluble in water, soluble in alcohol and oils.

Fresh, camphoraceous-minty, but rather weak odor of poor tenacity. In the undiluted state, the material has a sharp topnote. Bitter-minty, somewhat weedy taste.

This is not the most interesting of the three isomer ketones, but it finds a little use as a masking agent in industrial fragrances, "heavy-duty" household product fragrances, etc. It is also stable in soap and very stable towards oxidation. Since it is often available as a technical grade industrial chemical at a very low price, it has some advantage over the conventional and numerous fragrance materials of that odor type.

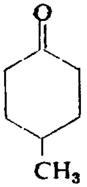
Prod.: 1) from Mentha Arvensis oil.

2) from Pennyroyal oil.
3) by dehydration of Pulegone, which is obtained e. g. as an intermediate in the production of synthetic Menthol.

26-602; 31-87; 31-85; 67-193; 67-198; 86-91; B-VII-17;

## 1972: 4-METHYL CYCLOHEXANONE

*para*-Methyl cyclohexanone.



$C_7H_{12}O = 112.17$

Colorless liquid. Sp.Gr. 0.92. B.P. 171° C.

Insoluble in water, soluble in alcohol and oils.

This isomer is the most pleasant-minty smelling of the three (see previous two monographs). Although not possessing a very natural minty note, it is not as harsh or camphoraceous as one usually observes in chemicals of this type. The tenacity is rather poor, but the odor is overall clean and refreshing.

This ketone could be used in fragrances for household products, in masking odors for industrial purposes, etc.

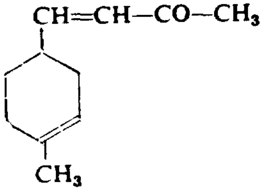
It is stable in soap and does not oxidize under normal conditions in functional products.

Prod.: by oxidation of *para*-Methyl cyclohexanol.

26-602; 31-87; 67-193; 67-199; 86-91; B-VII-18;

## 1973: 4-(1-METHYL-3-CYCLOHEXENYL)-3-BUTEN-2-ONE

Tetrahydro-*para*-methylbenzylidene acetone.



$C_{11}H_{16}O = 164.25$

Colorless or pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils.

Warm-herbaceous-spicy, penetrating and diffusive odor of Cumin-Caraway type.

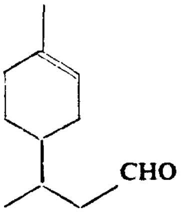
This ketone has been suggested for use in perfume compositions. Its main asset is its power and versatility. It blends well with Citrus oils, Lavender, Lavandin and other herbaceous oils, and it can introduce power and interesting notes to various floral fragrances, including Rose.

Prod.: by condensation of Acetone with *para*-Methyl-*3*-cyclohexene-carboxaldehyde.

(Sample: Dow Chem. Co. 1956).

## 1974: beta-(4-METHYL-3-CYCLOHEXENYL)-BUTYRALDEHYDE

*1*-Methyl-*para*-(*3*-Methylpropanal)-*1*-cyclohexene.
*3*-(*4*-Methyl-*3*-cyclohexenyl)-butanal.



$C_{11}H_{18}O = 166.27$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-floral odor with rosy-fruity undertones and moderate tenacity.

This material has – to the author's knowledge – not been offered commercially in practical amounts, but it was developed for use in perfumes, and its use was patented (patent recently expired).

It is probably still used as part or component of certain specialties and perfume bases, offered under trade name.

A number of related chemicals have been developed, many of them have been patented, – a procedure no longer very common and not generally considered of any value.

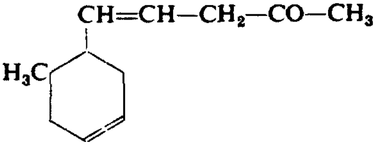
The title chemical is mentioned as one example of such material.

Prod.: from *d*- or *l*-Limonene, or Dipentene, with Carbon monoxide and Hydrogen as described in U.S. pat. 2.584.539 of Feb. 5, 1952.

See also U.S. pat. No. 2.710.825 of June 14, 1955.

## 1975: 1-(6-METHYL-3-CYCLOHEXENYL)-1-PENTEN-3-ONE

*6*-Methyl tetrahydrobenzylidene methylethyl ketone.



$C_{12}H_{18}O = 178.28$

Colorless or pale yellowish liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity-floral, Lavender-like odor of good tenacity. The odor has some pungency when undiluted, but becomes almost soft in sweetness when properly diluted.

This ketone has been suggested for use in perfume compositions of the heavy floral type, fruity-floral, Jasmin, Tuberose and modern-fruity fragrances.

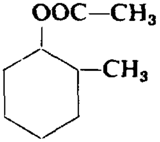
It is not always available under its proper chemical name, but it has experimentally been incorporated in perfumery specialties.

Prod.: by condensation of Methyl ethyl ketone and *6*-Methyl-*3*-cyclohexanecarboxaldehyde.

(Sample: Dow Chem. Co. 1956).

## 1976: 2-METHYL CYCLOHEXYL ACETATE

Hexahydro-*ortho*-cresylacetate.



$C_9H_{16}O_2 = 156.23$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful fruity and sweet odor of moderate to poor tenacity. The fruity notes are rather violent, not "natural", but may in proper dilution remind of Raspberry. There is a certain floralness of Jasmin character to the overall odor. The initial sharpness resembles that of Cedarleaf oil, camphoraceous-cineolic.

This ester, not often encountered in price lists, has found some use in perfume compositions, mainly in detergent perfumes and other fragrances for household products. It is comparatively stable, and a technical grade could be made available at reasonable price.

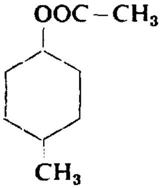
Generally speaking, however, one may say that this ester is of little interest to the perfume industry.

Prod.: by acetylation of *ortho*-Methyl cyclohexanol.

(See also 3-79).
(Sample: Dow Chem. Co.).

## 1977: 4-METHYL CYCLOHEXYL ACETATE

Hexahydro-*para*-tolylacetate.
Hexahydro-*para*-cresylacetate.



$C_9H_{16}O_2 = 156.23$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Intensely sweet, powerful, fruity odor of Raspberry-type with herbaceous-anisic undertones. Moderate tenacity. The odor bears some resemblance to that of Methyl-*para*-toluate.

This ester was introduced among a series of related chemicals, when the Cyclohexanol-family was a new field of perfume chemical research, and again brought into light in the early 1950's in the U.S.A.

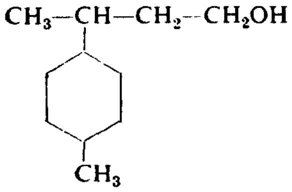
The subject material could find some use in low-cost Jasmin fragrances for household products and industrial perfumes for masking purposes. Its power and low cost encourage such uses, but its harshness prevents it from becoming a standard item in the more delicate floral creations. It blends excellently with the Ionones and with Benzylacetate, Amylsalicylate, Heliotropine, Safrole, etc. for inexpensive floral compositions, inexpensive Ylang-Ylang bases, etc.

Prod.: by direct esterification of *4*-Methylcyclohexanol.

(Sample: Dow Chem. Co. 1956).

## 1978: beta-(4-METHYL-CYCLOHEXYL)-BUTANOL

*3*-(*para*-Methyl cyclohexyl)-butanol-*1*.



$C_{11}H_{22}O = 170.30$

Colorless liquid. Solidifies in the cold.

Almost insoluble in water, soluble in alcohol and oils.

Semi-sweet, woody-rosy odor of moderate tenacity.

This alcohol is mentioned as one example of a series of chemicals developed from Dipentene or Limonene, by a process later applied to other Monoterpenes, often with interesting results.

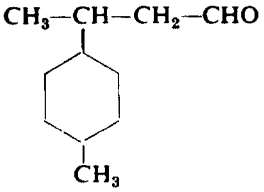
It has been suggested for use in perfume compositions, mainly soap perfumes, where its stability, low cost and olfactory versatility could make the material almost generally applicable. However, the common impression is that this chemical has limited odor value and does not offer enough of interesting note or power to justify a more general use of the alcohol.

Prod.: by hydrogenation of the aldehyde – see monograph: *beta*-(*4*-Methyl-*3*-cyclohexenyl)-butyraldehyde.

(See also U.S. pat. No. 2.556.150 of December 26, 1946).

## 1979: beta-(4-METHYL CYCLOHEXYL)-BUTYRALDEHYDE

3-(*para*-Methylcyclohexyl)-butanal.



$C_{11}H_{20}O = 168.28$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral, slightly green odor of moderate to good tenacity. The floral notes are rather nondescript, and the effect is more of a floral "lift" than truly an added floralcy.

This aldehyde represents another type of the series of chemicals developed from Limonene (or Dipentene). Most of these materials have never been offered commercially under their chemical name, but they have, in many cases, formed component of certain perfume bases and specialties.

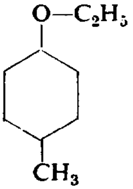
The patent covering its use in perfume compositions suggests a concentration of 1 to 3 % in the perfume, but the author would recommend a higher concentration – at least in modern detergent perfumes or other household product fragrances.

Prod.: by regulated hydrogenation of *beta*-(4-Methylcyclohexenyl)-butanal, (see monograph).

(See also U.S. patent No. 2.710.825 of June 14, 1955).

## 1980: para-METHYL CYCLOHEXYL ETHYLETHER

Hexahydro-*para*-cresol ethylether.



$C_9H_{18}O = 142.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Pungent-anisic, sweet odor of floral-herbaceous character and moderate tenacity.

This ether has been suggested for use in various low-cost fragrances for industrial purposes, household products, etc.

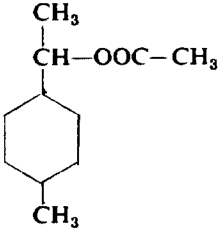
Its good stability and low cost are advantages, while its harshness and anisic character (which makes it far from versatile) are limiting factors to its application in perfumery.

Prod.: by controlled hydrogenation of *para*-Cresol ethylether.

3-286;
see also: 67-159;

## 1981: 4-METHYL CYCLOHEXYL METHYL CARBINYL ACETATE

Hexahydro-*para*-methyl styrallylacetate.
This chemical has been commercially marketed under the name of:
Methyl cyc*lohexenyl* methylcarbinyl acetate.



$C_{11}H_{17}O_2 = 181.26$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Floral-green, powerful and moderately tenacious odor.

This ester has been suggested for use in perfume compositions as a novel green note for floral compositions, introducing power, having stability and comparatively low cost, ready availability and other practical advantages.

However, it has not succeeded in surviving in the competition with the hundreds of other new perfume chemicals in the same overall odor character. At the present time (1968) it is not offered commercially from the regular suppliers of perfume chemicals.

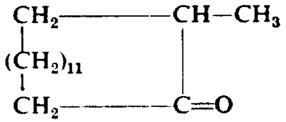
Prod.: by hydrogenation of *para*-Methylacetophenone, followed by Acetylation of the secondary alcohol.

3-182;

## 1982: 1-METHYLCYCLOPENTADECAN-2-ONE

*alpha*-Methyl cyclopentadecanone.

"*iso*-Muscone".



$C_{16}H_{30}O = 238.42$

Colorless liquid, viscous at room temperature, solidifying in the cold.

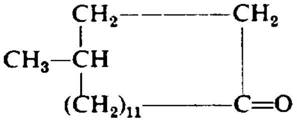
Sweet musky, pleasantly animal odor of excellent tenacity, weaker than Exaltone (see monograph: Cyclopentadecanone), but similar in odor type.

Since this material is normally prepared via Exaltone, and since it has no olfactory advantage over that ketone, there is little reason to believe that subject C-16-ketone will become a standard perfume chemical.

Prod.: by Methylation via the Sodio-derivative of Cyclopentadecanone.

31-107; 86-92;
see also: 4-89; 5-194;

## 1983: 4-METHYL CYCLOPENTADECANONE-1



$C_{16}H_{30}O = 238.42$

Colorless viscous liquid, solidifying in the cold.

Insoluble in water, soluble in alcohol and oils.

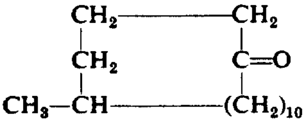
The odor of this isomer is musky, sweet and extremely tenacious, but it is still considered inferior in beauty, strength and naturalness when compared to Muscone.

Since this isomer does not have any significant economic advantage over the desirable Muscone, it is most conceivable that the subject material will remain of academic interest only.

Prod.: from the Thorium salt of 4-Methyl hexadecan dioic acid.

5-194; 31-107;

## 1984: 5-METHYL CYCLOPENTADECANONE-1



$C_{16}H_{30}O = 238.42$

Colorless viscous liquid, solidifying in the cold to a crystalline mass.

Insoluble in water, soluble in alcohol and oils.

Odor of Musk, sweet, extremely tenacious, but slightly weaker and not quite as sweet as that of Muscone (see that monograph).

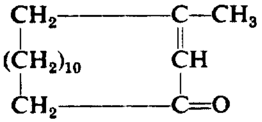
As long as this ketone does not even have economic advantages over Muscone, it is unlikely that it will be used in perfumery.

Prod.: via the Thorium salt of *5*-Methyl hexadecan dioic acid.

31-107;

## 1985: 3-METHYL CYCLOPENTADECENONE

"Muscenone".
This material is occasionally called:
*3*-Methylene cyclopentadecanone (confusing) in perfumery literature.



$C_{16}H_{28}O = 236.40$

Colorless viscous liquid, solidifying in the cold to a crystalline, colorless mass. B.P. higher than 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Delicate, but extremely tenacious musky odor, upon dilution developing more woody notes, not quite as soft and velvety as those of the Muscone, perhaps equal in power, but inferior in beauty.

This unsaturated ketone, which yields *dl*-Muscone upon hydrogenation, has been suggested as a modifier for the related ketones and lactones. It is equally expensive to prepare, and not as natural-musky in its character when compared to *l*-Muscone. Therefore, it is inconceivable that this ketone will become a common Musk at all.

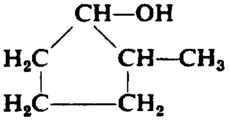
Prod.: by cyclization of *2,15*-Diketohexadecane with *N*-Methylaniline Magnesium bromide reagent.

4-89; 5-353; 86-101; 156-257;

## 1986: METHYL CYCLOPENTANOL

*2*-Methylhydroxycyclopentane.
Methyl cyclopentyl alcohol.

Note: The chemical referred to in perfumery literature is the secondary alcohol, while the tertiary alcohol: *1*-Methylcyclopentan-*1*-ol is quite commonly referred to in organic chemistry.



$C_6H_{12}O = 100.16$

Colorless mobile liquid. B.P. 149° C.

Very slightly soluble in water, soluble in alcohol and oils.

Green-leafy, herbaceous, slightly oily and "choking" odor of poor tenacity. Overall not nearly as natural as the alifatic alcohols.

This chemical has been suggested for use in perfumery, and when available at sufficiently low cost, it could find some use as part of masking odors for industrial purposes, etc.

Its odor type is not a rare one, and many low-cost material have similar type odor of much more attractive character. It is therefore unlikely that this alcohol, although plentifully available, will become a standard perfumery chemical.

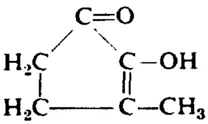
Prod.:

1) by reduction of 2-Methylcyclopentanone, which can be obtained by distillation of Methyladipic acid.
2) by Grignard type reaction upon Cyclopentene oxide.

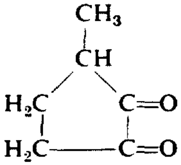
3-170; 67-86;

## 1987: METHYL CYCLOPENTENOLONE

"Cyclotene" (Dow Chem. Co.). (Glidden Co.).
"Corylone" (Givaudan-Geneva).
"Ketonarome" (Givaudan-Delawanna).
"Maple Lactone" (Th. Muhlethaler).
*alpha*-Methyl cyclopentenolone.
***2-Hydroxy-3-Methyl-2-cyclopenten-1-one.
**3-Methylcyclopentane-1,2-dione.



*** = "enol-form".



** = diketone form.

$C_6H_8O_2 = 112.13$ - or:

(Usually crystallizing with 1 Mol. water):

$C_8H_8O_2-H_2O = 130.15$

White or almost white crystalline powder or granular crystals. M.P. 106° C.

Soluble 2.5% in water, 3% in Glycerine, 14% in Propylene glycol, 25% in Ethylalcohol. Soluble in most perfume and flavor oils, but poorly soluble in terpenes and other hydrocarbons.

Sweet and very powerful, caramellic-spicy odor, described by different individuals with quite a variation of terms and phrases: Walnut – Maple – Licorice – Celery – Tobacco – etc. particularly when studied in the undiluted state by laymen. More reproducible evaluations are obtained when the material is studied at one percent strength in an odorless solvent.

The taste is intensely sweet, warm, slightly spicy, root-like, Walnut-Celery-like with Licorice-root and Maplesugar as the most common words of description. The odor type seems to change slightly with the concentration of the material.

This material, which has been marketed as a Hydroxyketone, belongs to a group of chemicals in which a tendency of "enolizing" is a common feature. The diketone structure (** above) is a form only recently ascribed to Cyclotene. The presence of a hydroxyl group is noticed by the perfumer or flavorist as a disadvantage when the material must be incorporated in an alkaline medium (not very common in flavors). The presence of one (or two) ketone group(s) is considered contributing factor to the unusual aroma power of this chemical.

Cyclotene (as it is most commonly called) is used sparingly in perfume compositions often in combination with Coumarin or Coumarin derivatives. It is an excellent fortifier for such materials in Lavender fragrances, New Mown Hay, "tabac" type fragrances, spicy bases, etc. It falls naturally into Celery seed oil, Lovage, Fenugreek, Tonka, Liatris, Flouve, etc.

It is, however, in flavor compositions that this material has found its truly extensive application.

In imitation Walnut and other nuts, Maple syrup, Rum (fixative), caramel, Butterscotch, spice blends and soup flavorings, wine flavor (Sherry wine, etc.) Coffee (as a modifier and smoothener), as a modifier in dentifrice mint flavors and mint candies, in licorice candy with Anise oil or Anethole, in Tobacco flavors as a modifier for coumarinic botanical extracts, Flouve oil, etc. as a fortifier for Coumarin and Methylcoumarins or Decalactone in Vanilla and Cream flavors, in numerous types of berry flavor, fruit flavor, etc.

The concentration used varies considerably with the type of effect desired, but it is normally about 5 to 30 ppm in the finished goods 20 ppm is quite common in candy, 35 ppm in syrups, highest in imitation Maple syrup.

The material discolors in contact with iron and in aqueous alkali. The "enol"-form of the material forms esters, some of which have been commercially marketed (see next).

G.R.A.S. F.E.M.A. No.2700.

Prod.: (many methods) e. g.: by ketonic hydrolysis of the corresponding Dicarboxylic ester.

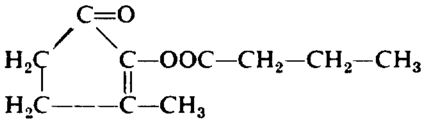
Also by halogenation of the Methylcyclopentanone, followed by hydrolysis of the resulting di-halide.

A considerable proportion of the world consumption is now manufactured by biological synthesis.

67-105; 86-92; 157-444;
see also: Dow Chem. Co. information sheet, June 1, 1948 (and later).

## 1988: METHYLCYCLOPENTENOLONE BUTYRATE

"Cyclotene butyrate".
The Butyric acid "ester" of the "enol" form of Methyl cyclopentenolone (see previous monograph).



$C_{10}H_{14}O_3 = 182.22$

Yellowish liquid, crystallizing in the cold.

Presumably not a well-defined chemical.

Slightly soluble in water, soluble in Propylene glycol, alcohol and many oils.

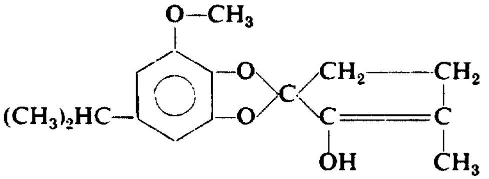
Powerful, creamy-caramellic, buttery odor of considerable tenacity. Sweet creamy-caramellic taste, slightly burning at concentrations higher than 30 ppm.

This material, occasionally offered commercially, has been used in flavor compositions, where a "Cyclotene" effect is desirable in combination with a buttery-creamy effect, particularly in imitation Butter, cream, Vanilla, and in Butterscotch, caramel, etc.

The material is not very stable, and any amount of free Butyric acid is likely to ruin the organoleptic picture of this material.

Prod.: by esterification of Methyl cyclopentenolone with Butyric acid, preferably under azeotropic conditions. The product is carefully washed acid-free.

## 1989: METHYLCYCLOPENTENOLONE-3,4-DIOXY-5-METHOXY-iso-PROPYLBENZENE



$C_{16}H_{20}O_4 = 276.34$

This rare chemical is included mainly for the sake of completing the picture of various additive products of Cyclotene.

It has been suggested for use in flavor compositions, and it is claimed to be of exceptional power and interesting sweetness, naturalness and versatility. Although it has not been expressly suggested for use in perfumes, the author would assume that this material could be an interesting perfume chemical, if it were made available in a reproducible quality and reasonable purity.

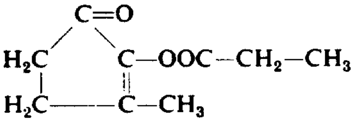
The author has no record of this material being commonly used in perfumes or flavors, but its components are highly interesting from a flavor study point of view.

Prod.: by condensation of Methylcyclopentenolone with 5-Methoxy-*iso*-divarinol, a Phenolether occurring in Beech wood tar. It can be prepared synthetically. The subject condensation product is a ketal of the substituted Catechol.

## 1990: METHYL CYCLOPENTENOLONE PROPIONATE

"Cyclotene propionate".

The commercial product has normally been marketed in the shape of a 50% solution in Propylene glycol. The solution would eventually separate crystals of Cyclotene.



$C_9H_{12}O_3 = 168.20$

Pale straw-colored viscous liquid, slowly separating crystals of Cyclotene.

Slightly soluble in water, miscible with Propylene glycol, alcohol and many flavor materials.

Powerful caramellic, somewhat sharp, Walnut-like intensely sweet odor of good tenacity.

Sweet caramellic, Walnut-like taste of considerable power.

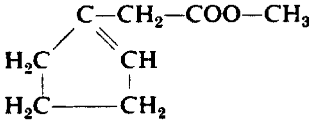
This ester (?) was probably prepared in an attempt to make available a more handy version of Cyclotene, specifically for flavor purposes. Its flavor character is, however, not significantly different from that of Cyclotene itself.

It seems that this material is of little interest as long as Cyclotene is available in the pure state.

Prod.: by esterification of Cyclotene with Propionic acid under azeotropic conditions.

## 1991: METHYL CYCLOPENTENYLACETATE

Cyclopentenylacetic acid, Methylester.
"Analine" (presumably main component).



$C_8H_{12}O_2 = 140.18$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Very diffusive and penetrating green-fruity odor of Apple-Pineapple and green-Citrus type. It bears some resemblance to the odor of Propyl-*iso*-valerate and Ethylcaproate, but is much fresher, completely free from fatty notes and, when freshly prepared or properly stored, also free from acrid-acid notes, resembling the Valeric ester notes.

This ester, very rarely offered commercially, is an excellent perfume and flavor chemical in the hands of the experienced creative perfumer or flavorist. Its versatility exceeds that of most other green or fruity materials, ranging from fruity Citrus notes to herbaceous Geranium or Clary Sage notes, refreshing when used in proper dilution, more green and less fruity in extreme dilution.

Its use in flavors is, naturally, much more interesting. It finds its way into imitation Apple, Pineapple, Pear, Gooseberry, Lemon, Lime, Rhubarb, etc. but should be used with utmost discretion and gentle touch. As a single material, its flavor is perceptible at concentrations of about 0.2 to 0.3 ppm, while it can be used at somewhat higher concentration when incorporated in a flavor base. Concentrations of 0.5 to 5 ppm are normal in finished products, highest in Pineapple.

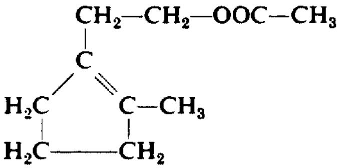
Prod.:

1) from Cyclopentanone via Reformatzsky reaction and esterification.
2) by condensation of Cyclopentanone with Malonic ester, followed by hydrolysis, decarboxylation and esterification.

3-10; 5-350; 67-113;
(material for studies: Givaudan Cie., Geneva).
The acetate of 2-Methylcyclopentenoic acid is also known (163-359).

## 1992: METHYL CYCLOPENTENYL ETHYLACETATE

*2*-Methylcyclopent-*1*-ene-*1*-acetic acid, Ethylester.



$C_{10}H_{16}O_2 = 168.24$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful, sweet, diffusive green-fruity odor of Pineapple type.

Sweet fruity, powerful Pineapple-type taste.

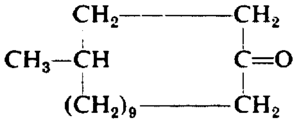
This ester is occasionally used in flavor compositions as a powerful Pineapple ingredient. It is also used in fruit complexes ("Tutti-frutti") etc. where power is requested.

Although rarely offered commercially, the ester is probably part of various flavor specialties and bases.

Prod.: from Methylcyclopentanone with Malonic ester, followed by hydrolysis, decarboxylation and esterification.

67-113;

## 1933: 4-METHYL CYCLOTETRADECAN-1-ONE



$C_{15}H_{28}O = 224.39$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, musky odor, but weaker and less "natural"-soft, slightly more "woody" than Cyclopentadecanone, the desirable isomer.

This isomer of Cyclopentadecanone is mentioned as an example of the many musks which, although very closely related to those presently preferred, do not compete favourably with the few, selected and preferred musks, some of which are present in natural musk.

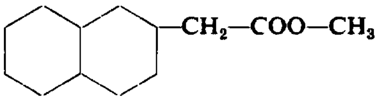
Although the natural Muscone has a Methyl side chain on a 15-membered Carbon-ring system, even the Nor-muscone is not as fine and natural as its higher homologue. The subject material is an isomer of Nor-muscone.

Prod.: e. g. from Citronellal plus Malonic acid plus Pyridine to make Citronellidene acetic acid, which is converted to *4*-Methyldodecane-*1,12*-dicarboxylic acid through several complicated steps.

31-107; 31-108;

## 1994: METHYL DECAHYDRONAPHTHYLACETATE

Decahydronaphthylacetic acid, Methylester. Decalin-*2*-carboxylic-*2*-acetic acid, Methylester.



$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-fruity, Pear-like odor, also with some resemblance to Benzylacetate. Good tenacity.

Sweet fruity taste of Pear-Bergamot type.

This ester is often offered under trade name, and it has been known to the perfume industry for a long time. In spite of this fact, the material has never achieved any significant position as a fragrance item, and it does not seem to offer any effect superior to those obtained with the conventional fruity-floral materials.

It has found a little use as a Jasmin modifier in low-cost soap perfumes and detergent fragrances, also as a modifier for Linalylacetate in Bergamot compositions, etc.

Prod.:

1) from Cyclohexanol by oxidation followed by alkali fusion and acidification. Finally esterification of the acid.
2) from *beta*-Decalone cyanhydrin plus Sodiocyanoacetic ester. Esterification of the acid.

31-127; 67-328;

## 1995: METHYL-2-DECENOATE

Methyl-*2*-decylenate.
Methyl-*beta*-heptylacrylate.
*3*-Heptylpropenoic acid, Methylester.

$CH_3(CH_2)_6CH{=}CH{-}COO{-}CH_3$

$C_{11}H_{20}O_2 = 184.27$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fruity, foliage-green odor of excellent diffusion and moderate tenacity.

This ester, comparatively rare in the price lists, has found some use in perfume compositions as part of topnote compositions with Citrus oils, Rose, Tuberose, alifatic aldehydes, etc. It gives interesting effects with the Hexenols and their esters, and it performs particularly well with Bitter Orange oil.

The material is quite powerful, and it is of some academic interest to study the ester along with the "metameric" ester, Decenyl acetate ("Roseate", I.F.F.). Although very different of odor type, the two esters produce highly attractive blends for further topnote creative work.

The ester has been suggested for use in flavor compositions, mainly in Citrus fruit and Melon flavors, or in minute traces in Strawberry. Since the title material is not listed in the American Federal Register or mentioned as G.R.A.S. by the F.E.M.A., it should not be incorporated in food flavors in the U.S.A.

Prod.: by direct esterification of *2*-Decenoic acid with Methanol, preferably using azeotropic conditions.

140-144;

## 1996: METHYL DECINCARBONATE

Methyl-*2*-undecynoate.

$CH_3(CH_2)_7C{\equiv}C{-}COO{-}CH_3$

$C_{12}H_{20}O_2 = 196.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, waxy-green, floral and slightly earthy odor of moderate tenacity. More waxy and more floral than the desirable Amyl heptincarbonate, which is generally considered the most "Violet" like of the series.

The heavy green notes of this ester makes it particularly suitable for Reseda (Mignonette) type bases, but it is also used in Violet, Cassie, Orris, Hyacinth, Jonquil, Narcisse, Tuberose and various floral fragrances where a sharp, leafy-green topnote is desirable.

The ester finds a little use in flavor compositions, in the comparatively rare types such as Violet and floral flavors, occasionally in certain types of Licorice candy flavoring.

The concentration is extremely low, usually about 0.1 to 20 ppm in the finished product.

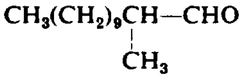
Prod.: from Methyl nonyl ketone with Phosphorous pentachloride to give the acetylenic compound. From this is prepared Undecyne with Potassium carbonate. Reaction with Sodium and Methyl chlorocarbonate yields the acid from which subject ester is prepared.

G.R.A.S. F.E.M.A. No.2751.

3-79; 4-89; 5-241; 103-295; 156-7;

## 1997: METHYL DECYL ACETALDEHYDE

*alpha*-Methyl dodecanal.
*10*-Methyldodecylaldehyde.
An isomer of Tridecanoic aldehyde (Aldehyde C-13).



$$CH_3(CH_2)_9CH(CH_3)—CHO$$

$C_{13}H_{26}O = 198.35$

Colorless oily liquid. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Dry-waxy, moderately powerful, but tenacious odor. In dilution quite refreshing, but lacks the Ambregris-like notes of the lower homologue (Methyl nonyl acetaldehyde).

This aldehyde, undoubtedly developed in search of other interesting "branched-chain" aldehydes after the success of MNA, has never attracted the perfumers to any marked degree. Its overall weakness when compared to the conventional aldehydes; its lack of character and versatility, are probably the main reasons for its falling into oblivion.

The lower homologue (see Methyl octyl acetaldehyde) has attracted much more interest.

The title material could be used with Oakmoss, Labdanum, Styrax, Galbanum, etc. in new variations of classic odor themes, but it could also give interesting effects in Pine needle fragrances, for which purpuse however, it would probably be too expensive. The useful concentration of the subject aldehyde is about 1 to 3% in the perfume oil.

Prod.: from Methyl decyl ketone via the glycidic ester by Darzens synthesis.

3-79; 163-49; 163-221;

## 1998: METHYL DECYL KETONE

Dodecan-*2*-one.
*2*-Dodecanone.
Decylmethyl ketone.

$CH_3—CO—CH_2(CH_2)_8CH_3$

$C_{12}H_{24}O = 184.32$

Colorless oily liquid. B.P. 246° C. Solidifies in the cold, melts at 21° C.

Insoluble in water, soluble in alcohol and oils.

Fruity, Orange-peel-like odor with sweet-waxy-floral notes, resembling part of the Orangeblossom-fragrance. There are fatty notes, but in suitable dilution only pleasantly fatty without any trace of rancid notes.

This ketone finds limited use in perfume compositions, partly as a modifier for alifatic aldehydes in fresh-floral-aldehydic fragrance types, partly as a variation note in Orange-blossom bases or Citrusy fragrances, It blends very well with the Aldehydes C-9, C-10, C-11 and C-12, also with the Citrus oils, Linalool, etc. It gives interesting effects with refined Labdanum products for Ambre bases, etc. and lends power to soap perfumes.

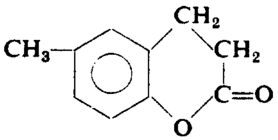
Prod.:

1) by oxidation of *secondary*-Dodecylalcohol.
2) by Grignard type reaction.
3) by Acetoacetic ester synthesis.

66-516;

## 1999: 6-METHYL DIHYDROCOUMARIN

"Methyl Melilotine" (Givaudan Corp.).
*6*-Methyl benzodihydropyrone.
*6*-Methyl hydrocoumarin.



$C_{10}H_{10}O_2 = 162.19$

White crystals. M.P. 81° C.

Soluble in most perfume oils, 1.5% soluble in alcohol, poorly soluble in water and Propylene glycol.

Warm haylike, heavy-sweet, herbaceous odor with a Coconut undertone and excellent tenacity. It has a much softer, Coconut-like character than Coumarin, and does not have the pungent-herbaceous, New Mown Haylike note of that material.

This lactone is used in perfume compositions where a more refined sweet-herbaceous effect is desirable, and where the Coconut-creamy effect is permissible. Therefore, it blends particularly well with Nonanolide in heavy floral fragrances, such a Gardenia and Tuberose, or the less floral types of Oriental, Chypre, Fougere, etc.

Milder variations of New Mown Hay may be obtained by the use of this material in place of Coumarin or Acetanisole or Anisaldehyde, all harsher than Methyldihydrocoumarin.

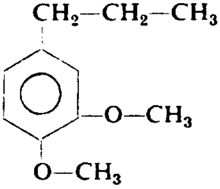
For particularly "creamy-floral" effects, sometimes highly desirable and difficult to achieve, this material offers good possibilities.

Prod.: by hydrogenation of *6*-Methylcoumarin (see that monograph).

106-246;

## 2000: METHYL DIHYDROEUGENOL

Dihydroeugenol methylether.
*3,4*-Dimethoxypropylbenzene.
*para-n*-Propylhydroquinone dimethylether.
Dihydromethyleugenol.



$C_{11}H_{16}O_2 = 180.25$

Almost colorless oily liquid. Sp.Gr. 1.04.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

This aromatic ether is rarely offered commercially, but has come into the limelight of perfumery since it was identified in natural products.

Its odor differs considerably from that of the conventional members of the Eugenol family in that it is only slightly spicy, not very powerful, but sweet and somewhat herbal in character. Its tenacity is fair and comparable to that of Methyleugenol.

No specific suggestions for its use have been made in writing, but it seems most conceivable that this ether will never gain a position of high importance in perfumery. As long as Eugenol remains strictly a natural derivative, not a true synthetic material, the availability of Clove leaf and Cinnamon leaf oils will monitor the cost and interest of the conventional Eugenol derivatives. The subject material can be produced via methods avoiding the Eugenol or the Clove leaf oil, but it seems unlikely that Eugenol will be produced via subject material if it ever will be produced a synthetic way.

Interest in Dihydroeugenol and its derivatives has apparently been encouraged by publications stating that these materials are less irritating to human skin than are the Eugenols. However, they can not substitute the Eugenols with respect to odor type or power in a fragrance.

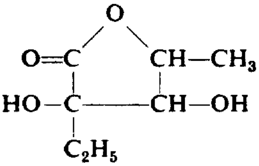
Prod.:

1) by Methylation of Dihydro eugenol with Dimethyl sulfate in weak aqueous alkaline solution. The Dihydro eugenol is prepared by catalytic reduction of Eugenol.
2) by Methylation of *4*-Propylpyrocatechol.
3) by controlled hydrogenation of Methyleugenol.

90-463; 156-162;

## 2001: 2-METHYL-3,4-DIHYDROXY-4-ETHYL-5-OXOTETRAHYDROFURAN

Methylethyl dihydroxy tetrahydrofuranone.



$C_7H_{12}O_4 = 160.17$

This chemical is briefly mentioned, although information about it is still very scarce.

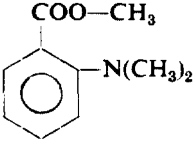
It represents a result of Japanese research work on the components of Soy sauce, and it has been named as one of the flavor factors in that product.

In view of its presence in such important food products, and since it is closely related to several other naturally occurring materials found in Pineapple and other widely different foods, there is reason to believe that the title material could become an important future flavor chemical. At this time, it is at least an important milestone in flavor chemistry research.

163-424;
(see also monograph: *2,5*-Dimethyl-*4*-hydroxy-*3*(*2H*)-furanone). No. 1025.

## 2002: METHYL-N,N-DIMETHYL-ANTHRANILATE

*N,N*-Dimethylanthranilic acid, Methylester.



$C_{10}H_{13}NO_2 = 179.22$

Colorless or very pale straw-colored oily liquid. B.P. 233° C.

Almost insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Musty-sweet, deep-floral and fruity odor of good tenacity. It bears some resemblance to the odor of oil from Orange leaf water and Orange flower water, not really a refreshing odor.

This rare ester has been suggested for use in perfume compositions as a modifier for the conventional Anthranilates and *N*-Methylanthranilates in floral and Oriental fragrance types. It gives interesting variations but appears rather dry as compared to the common esters.

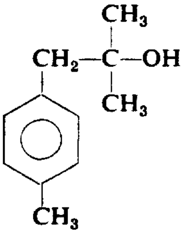
Prod.:

1) from Anthranilic acid, methylated by Willstätter reaction, followed by esterification.
2) from Betaine by heating with Sodium methoxide in Methanol.

68-582;

## 2003: para-METHYL DIMETHYLBENZYLCARBINOL

Dimethyl-*para*-tolylcarbinol.
*para*-Tolyl dimethylcarbinol (misleading name).
*alpha,alpha,para*-Trimethyl phenylethylalcohol.
*para*-Methyl-DMBC.



$C_{11}H_{16}O = 164.25$

Colorless, slightly viscous or oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Mild-green and floral, slightly balsamic, very tenacious odor of pleasant, natural overall character.

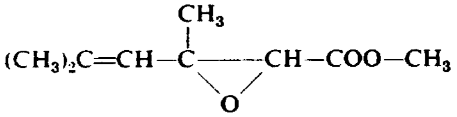
This "carbinol", which could be classified as a higher homologue of the "DMBC", is rarely offered commercially, perhaps mainly because it will inevitably be more expensive than the common DMBC, and it has apparently been difficult to convince the perfumers that it has advantages and virtues not found in the Dimethyl benzylcarbinol. Its green undertones combined with a distinct floralness are features found in the highly appreciated and valued Phenylethyl dimethylcarbinol (Dimethyl phenylethyl carbinol) and it is tempting to use such fine combinations in the more delicate floral fragrances e. g. Muguet, Lily, Peony, Rose, Lilac, etc. It performs particularly well in Lilac which, unfortunately, is generally forced into a class of fragrances for which the customer applies a very low price limit.

The material is stable in soap, also stable against oxidation, and it blends excellently with practically all the conventional perfume materials for floral and green-herbaceous or Oriental-balsamic notes.

Prod.: by Grignard type synthesis from Tolyl magnesium bromide plus Acetone.

## 2004: METHYL-3,5-DIMETHYL-2,3-EPOXY-4-HEXENOATE

"Glycidate M-116" (U.O.P. Fragrances).
Methyl methyl-*secondary*-butenylglycidate.



$C_9H_{14}O_3 = 170.21$

Colorless or pale straw-colored oily liquid.

Slightly soluble in water, soluble in alcohol, Propylene glycol and perfume and flavor oils.

Sweet-caramellic odor with a mildly fruity undertone.

Strawberry-Pineapple-like, fruity-malty taste with a faint background of sweet berry-like character.

This unusual ester, developed by the Trubek laboratories in 1958, has been marketed under the name of Glycidate M-116 by that company and its later owners for 10 years without any sign of outstanding success. Whatever the reason may be, it shows how difficult it is, at times, to launch and make popular an entirely unknown chemical just by tempting the potential customers to try it in their products or novel developments. The author can see no reason why this material should not have become a generally accepted and commonly used flavor and fragrance chemical by the time of editing this monograph (1968), but perhaps the timing was unfortunate. The material appeared just when Maltol (Palatone) and Cyclotene had their come-backs in perfumes and flavors, and the new experimenting with these materials seemed to dominate all evaluations of other and similar materials.

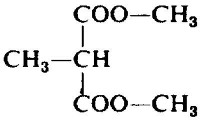
This glycidate could find use in imitation Strawberry, in Caramel, treacle, Butterscotch, Maple, Nut, Vanilla, Pineapple, Raspberry, etc. The normal use-level would be equivalent to 20 to 50 ppm in the finished product.

Prod.: from Mesityl oxide plus Ethyl chloroacetate and Sodium methylate by the conventional Glycidic ester synthesis.

See also: Ethyl methyl *iso*-hexenylglycidate. No. 1298.

## 2005: METHYL DIMETHYLMALONATE

Methylmalonic acid, Dimethylester.
Methyl methylmalonate.
Dimethyl-methylpropane dioate.
Dimethyl-*iso*-succinate.



$$\begin{array}{l} \qquad \mathrm{COO-CH_3} \\ \qquad | \\ \mathrm{CH_3-CH} \\ \qquad | \\ \qquad \mathrm{COO-CH_3} \end{array}$$

$C_6H_{10}O_4 = 146.15$

Colorless liquid. Sp.Gr. 1.03. B.P. 179° C.

Slightly soluble in water, soluble in alcohol and oils.

Mild winey-fruity, ethereal odor of poor tenacity.

Sweet-winey, slightly fruity taste.

This ester has been suggested for use as a diluent in certain types of perfume, in which a mild, fruity odor is acceptable.

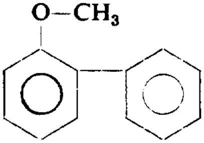
It may dilute a Rose base to the point where its odor becomes more agreeable to a customer, and it can therefore serve the purpose of adjusting powerful bases to odor levels acceptable by non-perfumers. The effect is sometimes referred to aş "blending", but that term is normally applied to materials of a different nature and effect.

Prod.: by condensation of Ethylpropionate with Ethyloxalate.

66-966; 160-1086; B-II-628;

## 2006: METHYL DIPHENYLETHER

*ortho*-Phenylanisole.
*ortho*-Phenyl methylphenylether.
*2*-Methoxy biphenyl.



$C_{13}H_{12}O = 184.24$

Colorless crystalline mass, melting to a colorless oily liquid. M.P. 29° C. B.P. 274° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, green-rosy odor of good tenacity. Some observers find a fruity note in this odor. It is mild enough, that it can be incorporated in fruity fragrances and actually support that type of odor by blending action.

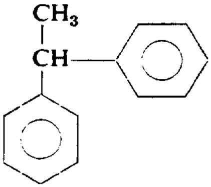
This inexpensive and simple ether is, surprisingly enough, completely unknown in certain perfumery circles. It is manufactured by very large chemical manufacturers, and regularly offered by well-known perfume chemical suppliers, yet missing from many a perfumer's shelf.

It finds good use in soap perfumes, where its low cost and good stability make it very applicable and practical. Its odor type makes it particularly suitable for Rose fragrances, Geranium, Lavender, Pine needle and mild woody odors. It blends well with the conventional Cyclohexanol-derivatives.

106-247; 160-872;

## 2007: METHYL DIPHENYL METHANE

*asymmetric, alpha-alpha*-Diphenylethane.
*1,1*-Diphenylethane.
*alpha*-Methyl ditane.



$C_{14}H_{14} = 182.27$

Colorless liquid. B.P. 270° C. Sp.Gr. 0.99.

Practically insoluble in water, soluble in alcohol and oils.

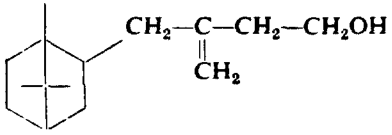
Sweet, mildly green-rosy, somewhat "metallic" but overall pleasant odor of good tenacity. Not quite as harsh as Diphenylmethane, and not as powerful as Diphenyloxide, but stronger than Methyl diphenylether.

The title material has occasionally been used as an inexpensive perfume material for low-cost fragrances in functional products where exceptional stability is required. When it has been available at a cost near that of Diphenyloxide and Diphenylmethane, it has had fair chances of being used as a modifier in Rose and Hyacinth type fragrances for industrial products, household products, etc.

Prod.: by Friedel-Craft's reaction on Styrene plus Benzene (with Aluminum chloride).

See also: Diphenylmethane.

## 2008: 3-METHYLENE-4-BORNYLBUTANOL



$C_{15}H_{26}O = 222.37$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

This alcohol represents another type of many chemicals developed in search of new and interesting Sandalwood odors. There are now several types, but most of them are based upon Camphenol or Camphanol with an alifatic or olefinic chain, or with a Cyclohexanol substitution at the hydroxyl radicle in the terpene alcohol.

Most of these materials are sold under trade names, and a few have become quite successful.

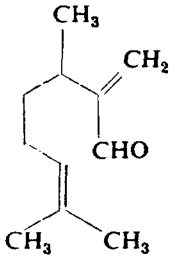
The title material is used as partial substitute for Sandalwood oil which is still (Sept. 1968) unreasonably expensive for liberal use in ordinary perfumery. However, it lacks the intense sweetness in the woody notes, and the almost animal-heavy undertones of natural Sandalwood oil.

163-360;

see also: *iso*-Bornyl methoxy cyclohexanol
*3*(*iso*-Camphenyl-*8*)-*2*-methylpropanol-*1*
*3*-(*iso*-Camphyl-*5*)-cyclohexanol.

## 2009: alpha-METHYLENE CITRONELLAL

*2*-Methylene-*3*,*7*-dimethyl-*6*-octen-*1*-al.



$C_{11}H_{18}O = 166.27$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

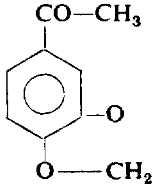
Sweet and refreshing, citrusy-herbaceous odor of moderate tenacity.

This aldehyde, rarely offered under its chemical name, has been suggested for use in perfume compositions for its powerful and refreshing, yet sweet effect which blends excellently with Bergamot notes. Supported by the new and very reasonably priced Ethyl linalool and Ethyl linalyl acetate, etc., this aldehyde can introduce rich Bergamot-undertones in a very economical way.

The aldehyde is pleasantly free from the harshness of Citronellal, and it does not seem to resinify quite so easily, although it suffers from the usual drawbacks found in unsaturated terpenoid aldehydes.

## 2010: 3,4-METHYLENE DIOXYACETOPHENONE

Acetopiperone.
Sometimes called:
Methyl piperonyl ketone.



$C_9H_8O_3 = 164.16$

Colorless or white crystals. M.P. 89° C.

Almost insoluble in water, soluble in alcohol and oils.

Heavy, sweet-floral and warm-herbaceous odor of considerable tenacity. The herbaceous notes tend to be spicy at high concentration, while lower concentrations only introduce sweetness, support floral notes and extend the fixation.

This material, although simple from a chemical point of view, is rarely offered commercially under its proper chemical name. It is used in certain perfume specialties and bases, and is usually manufactured by the user.

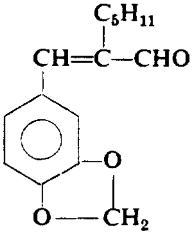
Literature has described the material as having a "Caraway type" odor, but the author has observed no such odor in the samples evaluated so far.

Prod.:

1) from Piperonylic acid plus Acetic acid vapors at high temperature over catalyst (Thoria, e.g.).
2) from *alpha*-Methylpiperonylic acid by oxidation.

163-360; 3-190; 68-753;

## 2011: 3,4-**METHYLENEDIOXY**-alpha-n-**AMYLCINNAMIC ALDEHYDE**



$C_{15}H_{18}O_3 = 246.31$

Pale yellowish oily and viscous liquid.
B.P. over 320° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Very mild oily-floral, warm odor of considerable tenacity.

This aldehyde was evidently developed with the hope in mind that Heliotropine would offer a much superior base material for the condensation product than Benzaldehyde which had already yielded one of the most successful perfume chemicals ever produced. But the resulting aldehyde was not very encouraging, and it is rarely offered under its proper chemical name, actually unknown to most perfume laboratories.

Perhaps superior to Amylcinnamic aldehyde with respect to tenacity and fixative effect, this aldehyde does not seem to "bloom" upon dilution the way ACA does. And that is a major drawback. It is furthermore floral without being specifically Jasmine-like, in fact, it does not resemble any particular natural product.

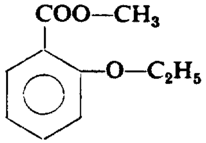
Prod.: by condensation of Heliotropine and Heptaldehyde in weak aqueous alkaline solution.

86-92;

## 2012: **METHYL**-ortho-**ETHOXYBENZOATE**

*ortho*-Ethoxy methylbenzoate.
Methylsalicylate ethylether.

Note: A material, known as "Spirosal", *beta*-Hydroxyethylsalicylate, is occasionally confused with subject material. Spirosal has only medicinal application. The name "Methyl-*beta*-ethoxysalicylate" is also confusingly used in perfumery literature.



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid.

B.P. 254° C. Sp.Gr. 1.13.

Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, slightly spicy-floral odor of good tenacity. The floral notes resemble Rose, Tuberose, Gardenia, while the spicy-fruity notes are of the Grape-Wintergreen theme.

The taste is warm, sweet and somewhat resembling that of Blackcurrant.

This ether-ester is occasionally used in perfumes as a modifier for Methyl- and Ethylbenzoate in heavy florals. Yet, it gives interesting effect and good power in Rose compositions for soap.

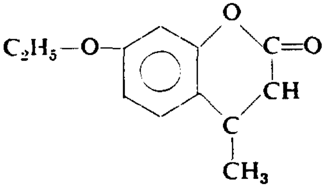
It has been suggested for imitation Blackcurrant and other berry type flavors. It blends excellently with the Anthranilates, lending an often needed warm sweetness and good fixation.

Prod.: by Ethylation of Methylsalicylate with Diethylsulfate in weak aqueous alkali.

34-787;

## 2013: 4-METHYL-7-ETHOXYCOUMARIN

"Maraniol" (Givaudan Corp.).
"Madescol" (Dr. Schmitz Co.).
Ethoxyresocyanin.
*beta*-Methylumbelliferone ethylether.



$C_{12}H_{12}O_3 = 204.23$

White crystal needles. M.P. 114° C.

Very slightly soluble in water, 1.5% soluble in alcohol, slightly soluble in most perfume and flavor oils.

Deep-sweet, Walnut-Celery-like, warm and tenacious odor with emphasis on the Nut-like character.

Maple-Nut-like taste, very sweet, slightly Celery-like and with an overall resemblance to Fenugreek. However, without the enormous radiance and power of that natural material.

This interesting Lactone has been known for many decades, but is still missing in many perfume laboratories. One reason for its lack of popularity may be found in the very poor solubility, a fact which inevitably will annoy the experimenting perfumer. The power of the material is usually of such magnitude, that it will compensate for the rather low level of concentration necessary to keep Maraniol in solution.

It offers very interesting variations of the Coumarin-Fougère theme, and gives novel effects in Chypre when used in place of part of the Coumarin intended for a Chypre. It forms obviously a warm and solid background in those fragrances where Celery seed oil is used as a topnote material, and it supports tobacco notes, New Mown Hay, etc. It is, however, in flavors that this material shows its more interesting versatility.

It is used in all types of imitation Nut, Walnut, Coconut, in Maple and Maple-Walnut, Pecan, as a sweetener in Peanut butter, as a fixative in Rum flavors, and it is often used in combination with Resorcinoldimethylether, Hydroquinone dimethylether, Nonanolide, Decanolide, Cyclotene, substituted Coumarins, Furfural derivatives, etc.

Its high boiling point makes it an excellent fixative for flavors in baked goods, etc.

It is interesting to note that unconfirmed reports place a Methylumbelliferone ethylether as a component of Fenugreek seed. The close relationship between that Lactone ether and subject material should encourage further olfactory-chemical studies.

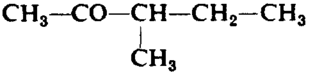
Prod.:

1) from Diketene plus Resorcinol with sulfuric acid to produce 4-Methyl-7-hydroxycoumarin. Ethylation produces subject material.
2) from Resorcinol plus Ethylacetoacetate, followed by Ethylation.

4-84; 7-179; 21-272; 27-191; 106-228; 156-133; 69-880;

## 2014: METHYL ETHYL ACETONE

Methyl-*secondary*-butyl ketone.
*alpha-alpha*-Methylethylacetone.
*3*-Ethyl-*2*-butanone.
*3*-Methylpentan-*2*-one.



$$CH_3-CO-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-CH_3$$

$C_6H_{12}O = 100.16$

Colorless mobile liquid. B.P. 118° C.
Sp.Gr. 0.81.

Slightly soluble in water, miscible with alcohol and oils.

Very diffusive, minty-camphoraceous "bitter" odor of considerable penetrating effect.

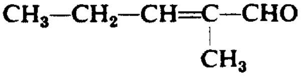
This ketone has occasionally been used as a masking agent in industrial perfumes or masking compositions for industrial or household products. It covers or distracts from the kerosene odor, a common problem in many cleansing products, but it is not an odor generally accepted by the public, although it may be preferred to the kerosene odor.

Prod.:
1) by Grignard type synthesis.
2) from Methyl ethyl acetoacetic ester.

26-600; 31-91; 61-67; 66-516; 66-518; B-I-693;

## 2015: alpha-METHYL-beta-ETHYL ACROLEIN

*2*-Methyl-*2*-pentenal.
"Homo Tiglic aldehyde".
*2,4*-Dimethyl crotonaldehyde.
"*iso*-Hexenal".



$$CH_3-CH_2-CH{=}\underset{\displaystyle CH_3}{\underset{|}{C}}-CHO$$

$C_6H_{10}O = 98.15$

Colorless mobile liquid. B.P. 137° C.
Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, "gassy"-green and slightly fruity odor of poor tenacity.

This aldehyde has been suggested for use in perfume compositions as part of novel green topnote complexes. It has also been used to a minor extent in the reconstruction of certain essential oils.

Its type of greenness, however, is not nearly as attractive as those of the conventional Hexenals, and it is not likely that the title aldehyde will become a common perfumery item.

The aldehyde has found some use in the reconstruction of Onion volatile oil, in which it has been identified as a natural component. It has also been identified as a natural component of Coffee bean (before roasting), and furthermore in the volatile components of roasted Coffee bean.

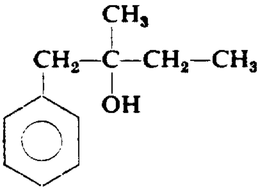
The title aldehyde has been synthesized mainly for the purpose of using it in reconstituting the aroma in dry Coffee extracts ("Instant Coffee") and in Onion flavors. However, the material forms only a minor part of the very complex and delicate aroma-picture of Coffee.

Prodl.: From Propionaldehyde by self-condensation (Aldol-condensation).

66-503; 157-390; 157-443; 158-143; B-I-735;

## 2016: METHYL ETHYL BENZYL CARBINOL

Benzyl ethyl methyl carbinol.
Benzyl methyl ethyl carbinol.
*2*-Methyl-*2*-hydroxy-*1*-phenylbutane.
*2*-Methyl-*1*-phenylbutan-*2*-ol.
"Homo-DMBC".



$C_{11}H_{16}O = 164.25$

Colorless, slightly viscous liquid.
Sp.Gr. 0.97. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar green-floral, rather dry, mossy, almost leather-like odor (not phenolic, but sweet-leather, cured skins) overall milder than Dimethyl benzyl carbinylacetate.

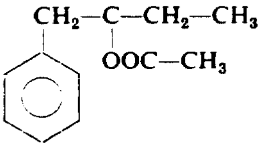
This tertiary alcohol is used in perfume compositions, partly for delicate floral fragrance types, partly for green-mossy or Oriental types. It blends excellently with Oakmoss and Vetiver, but also forms soft and natural-green floral notes with Heliotropine, Anisylacetate etc. in Lilac or Lindenblossom. It is an excellent blender/background note for Honeysuckle.

Prod.: by Grignard type synthesis from Benzyl magnesium bromide plus Methyl ethyl ketone.

34-161; 37-515; 68-501; 156-76;

## 2017: METHYL ETHYL BENZYL CARBINYL ACETATE

Benzyl ethyl methyl carbinyl acetate.
Benzyl methyl ethyl carbinyl acetate.
"Homo-DMBCA".



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-green and floral, moderately tenacious odor. Sometimes described in literature as "leathery", however, the author believes that such description must be based upon observations on impure material.

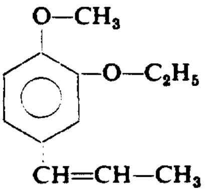
This ester finds a little use in perfume compositions for Lilac, Peony, Honeysuckle, Lindenblossom, Appleblossom, etc., mostly in delicate florals. Appleblossom is – in Nature – an extremely delicate fragrance, but has – for some inexplicable reason – been depicted by perfumers as a shockingly harsh and pungent "odor" based upon Phenylacetaldehyde, Anisaldehyde, etc. Maybe because the customers have demanded "more power" repeatedly and thus contributed to the destruction of the delicate Appleblossom fragrance. It could also be a result of misinterpretation on behalf of many perfumers when they add pungency instead of introducing power in the creation. There is a distinct difference between pungency and power.

Prod.: by direct esterification of the carbinol with Acetic acid under azeotropic conditions. Esterification with the anhydride or under acid conditions (mineral acid addition) is not recommended for tertiary alcohols.

34-161; 34-162;

## 2018: METHYL ETHYL-iso-EUGENOL

A somewhat confusing name for:
*4*-Propenylcatechol methyl ethylether.
Ethoxy-*iso*-chavibetol.
An isomer of Ethyl-*iso*-eugenol.



$C_{12}H_{16}O_2 = 192.26$

White or colorless crystal needles.

Practically insoluble in water, slightly soluble in alcohol, soluble in warm alcohol and in most oils.

This phenolether has come out of extensive research in the Vanillin field. It appears to be one of the least interesting products of this family, but it is included in this work for the sake of completion and clarification on certain common cases of confusion in these chemical names.

Its odor is very weak, more medicinal than sweet, and its taste is also mostly medicinal, with no power of sweetness.

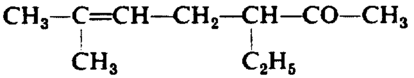
It could find use as a perfume fixative in Carnation and spice blends, but its cost would be prohibitive for such application.

Prod.: by ethylation of isomerized Betel-phenol (*iso*-Chavibetol).

(See also: Propenyl guaethol) 2649.
(See also: 72-70).

## 2019: METHYL-3-ETHYL HEPTENONE

*alpha*-Ethyl-*alpha*-methylbutenyl acetone.



$$CH_3-\underset{\displaystyle CH_3}{\overset{}{C}}=CH-CH_2-\underset{\displaystyle C_2H_5}{CH}-CO-CH_3$$

$C_{10}H_{18}O = 154.25$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, fruity-green, herbaceous and sweet odor of moderate tenacity. There is an almost Basil-like spiciness or anisic note of very natural character in this odor.

This ketone, only recently brought on the market as a regularly available chemical, has been suggested for use in perfume compositions particularly where power, sweetness and fresh-fruity notes are wanted or acceptable.

It blends excellently with Lavender and Lavandin, with the herbal oils of Oriental fragrance types, Opopanax and Labdanum, Citrus oils etc. – a very versatile fragrance chemical.

It gives interesting novel notes in sophisticated Pine fragrances and Fougères, and in discrete amounts it may add power to floral notes of the Lily, Jasmin or Gardenia type.

In the author's opinion, a very promising perfume chemical.

Prod.: (several methods) e. g. from Ethyl-*2*-ethyl-*2*-prenylacetoacetate by decarboxylation.

(Sample: Hoffmann-laRoche, Inc.).

## 2020: METHYL ETHYL KETONE

*2*-Butanone.
"Ketone C-4".
Ethyl methyl ketone.
"M.E.K." (commercial abbreviation).

$CH_3-CO-CH_2-CH_3$

$C_4H_8O = 72.11$

Colorless mobile liquid. Sp.Gr. 0.81.
B.P. 80° C.

30% soluble in cold water, 20% in hot water. Will dissolve 12% water at room temperature.

Miscible with alcohol, Propylene glycol, Glycerin and oils.

Ethereal, slightly nauseating odor, not exactly pleasant.

This ketone is probably not used in perfumery.

It finds limited use in flavor compositions, particularly in imitation Coffee (since it has been identified in roasted Coffee volatiles). The concentration used in such flavor types is rather high, about 200 to 250 ppm.

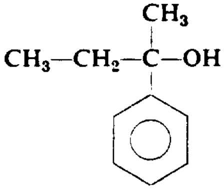
Prod.:
1) by oxidation of *secondary*-Butylalcohol.
2) from Methyl acetoacetate with diluted sulfuric acid.
3) by fermentation.

G.R.A.S. F.E.M.A. No.2170.

31-84; 31-80; 100-677; 160-884;

## 2021: METHYL ETHYL PHENYL CARBINOL

Ethyl methyl phenyl carbinol.
Phenyl methyl ethyl carbinol.
*1*-Methyl-*1*-phenylpropanol-*1*.
"*iso*-DMBC".



$C_{10}H_{14}O = 150.22$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

This carbinol, not nearly as common or readily available as its isomer, Dimethylbenzylcarbinol, finds a little use in perfume compositions.

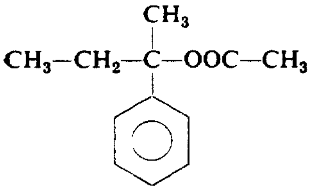
Its odor is somewhat similar to that of DMBC, however, more dry, slightly woody-camphoraceous, overall not so floral. It has a pleasant greenness and blends well with Oakmoss, Amylsalicylate, herbaceous oils, Terpineol, Heliotropine, Coumarin, etc., but does not point in any specific floral direction.

The acetate (see next) is much more useful and versatile.

Prod.: by Grignard type synthesis from Phenylmagnesium bromide plus Methyl ethyl ketone.

## 2022: METHYL ETHYL PHENYL CARBINYL ACETATE

Ethyl methyl phenyl carbinyl acetate.
Phenyl methyl ethyl carbinyl acetate.
*1*-Methyl-*1*-phenyl propylacetate.
"*iso*-DMBCA".



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-floral, slightly green and fruity odor of fair to good tenacity.

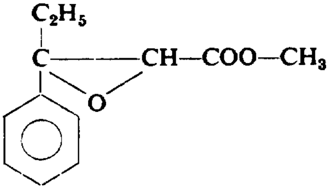
This ester has some of the virtues of the more popular Dimethyl benzyl carbinyl acetate, but it gives interesting variation to that theme, or it can be used separately for more unusual floral creation, such as Freesia, Gardenia, Lily, Narcissus, etc. The ester blends very well with the conventional floral materials such as Benzylacetate, Tolyl acetate, Amylcinnamic aldehyde, Heliotropine, Phenylethyl esters, etc.

Prod.: by azeotropic type esterification of the carbinol with Acetic acid and a catalyst.

28-608;

## 2023: METHYL ETHYL PHENYLGLYCIDATE

Methyl-*2,3*-epoxy-*3*-ethylhydrocinnamate.
The Methylester of Ethylphenylglycidic acid.
NOTE: Do not confuse with *para*-Methylethyl phenylglycidate (see next).



$C_{12}H_{14}O_3 = 206.24$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet caramellic-fruity, ethereal odor of moderate to poor tenacity. Sharper and less fruity, more caramellic-ethereal than Ethyl methyl phenylglycidate (so-called Aldehyde C-16).

Sweet caramellic-fruity taste, weaker than EMPG).

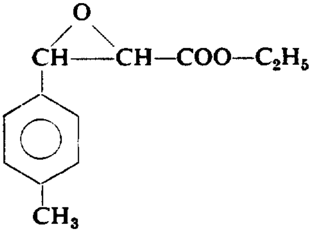
This ester, which could be called the "reverse ester" of Ethyl methyl phenylglycidate, has failed to attract interest among the perfumers and flavorists, partly because it is very rarely offered commercially, partly because most observers agree, that EMPG is superior with respect to fruity Strawberry notes.

Prod.: from Propiophenone plus Methylmonochloroacetate with Sodamide condensing agent (or Sodium methoxide).

(See also monograph: Ethyl methyl phenyl glycidate). No. 1306.

## 2024: para-METHYL ETHYL PHENYL GLYCIDATE

Ethyl-*2,3*-epoxy-*3*-(*para*-tolyl)-propionate.
*para*-Methyl-E.P.G.
Occasionally confused with Methyl ethyl phenyl glycidate, see previous monograph. The title material is more common than the previously mentioned one.



$C_{12}H_{14}O_3 = 206.24$

Colorless oily liquid. B.P. 271° C.
Sp.Gr. 1.09.

Practically insoluble in water, soluble in alcohol and oils.

Very sweet, powerfully fruity, Raspberry-like odor of good tenacity. Fresher, sweeter than Ethyl methyl phenyl glycidate, and more fresh-fruity, less caramellic than Ethyl phenyl glycidate.

The ester is used in perfume compositions as a fruity and sweet odorant, a modifier of the more conventional glycidates, and in larger amounts, in fruity perfume bases under various trade names, often referring to Raspberry.

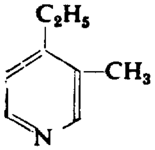
In concentrations below 20 ppm, the taste is intensely sweet, Raspberry-like and quite pleasant. Slightly more "Cherry-pit-like" than Ethyl methyl phenyl glycidate, fresher, less pungent.

The material is *not* specifically mentioned in the American G.R.A.S. list.

Prod.: from *para*-Tolylaldehyde plus Ethyl monochloroacetate with Sodamide or Sodium ethoxide as condensing agent.

163-219;

## 2025: 3-METHYL-4-ETHYL PYRIDINE



$C_8H_{11}N = 121.18$

Colorless to pale straw-colored oily liquid. Almost insoluble in water, soluble in alcohol and oils.

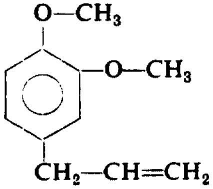
Sweet-herbaceous, slightly spicy odor of considerable diffusive power, but only moderate to poor tenacity. Weaker and greener than the *3*-Ethyl-*4*-methyl pyridine (see monograph) and not earthy.

This alkyl-substituted Pyridine is commercially available and has occasionally been suggested for use in perfume compositions. It blends well with Lavender and Lavandin, Amylsalicylate, Labdanum, etc., but its most interesting effects are those in flower absolute imitations and artificial essential oils, where traces can add some of the missing "natural" greenness to the base.

Sample: Reilly Tar & Chemical Comp., Indianapolis, U.S.A.

## 2026: METHYL EUGENOL

Eugenol methylether.
*4*-Allyl veratrole.
*1,2*-Dimethoxy-*4*-allylbenzene.



$C_{11}H_{14}O_2 = 178.23$

Almost colorless oily liquid. Sp.Gr. 1.04. B.P. 249° C.

Practically insoluble in water, soluble in alcohol and oils.

Peculiar musty-tealike, warm and mildly spicy, slightly earthy, tenacious odor. The warm notes are mostly herbaceous, the spicy notes very subdued, and there is an overall resemblance to notes of Ginger and Tea.

The taste is somewhat dry, tealike, warm and mildly spicy.

This phenolether, widely occurring in Nature, is used in many perfume types. Let it be said at once, it is in no way a substitute for Eugenol, but it has its own peculiar, delicate spiciness.

Its main role in perfumes is that of introducing a warm background and it can do so in floral as well as in herbaceous fragrance types, in Oriental-spicy bases, etc. It is a frequently occurring component in variations of the "Origan" theme, and it forms a pleasant background in Ylang-Ylang bases, Carnation, Lilac, Leather notes, Lavender and Clary Sage types, Bay-Rum and Men's spicy colognes, etc.

It blends well with the "carbinols", herbaceous oils, spice oils, etc. and does not tend to discolor under normal composition conditions. The material is also used in flavor compositions, mainly as a modifier in spice blends, to support Ginger-like notes, etc. Its low rate of volatility makes it suitable for flavors for baked goods, etc.

The normal concentration will be about 5 to 15 ppm in the finished product.

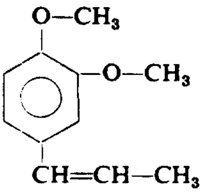
G.R.A.S. F.E.M.A. No.2475.

Prod.: by Methylation of Eugenol with Dimethyl sulfate in aqueous alkali. The Eugenol may be derived from Clove leaf oil.

4-50; 4-89; 34-1116; 77-198; 90-464; 106-248; 160-1276; 156-162;

## 2027: METHYL-iso-EUGENOL

*iso*-Eugenol methylether.
*4*-Propenyl veratrole.
*1,2*-Dimethoxy-*4*-propenylbenzene.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid, solidifying in the cold. M.P. 6° C.*) B.P. 270° C. Sp.Gr. 1.05.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and warm, mild floral-tealike, very slightly spicy and very tenacious odor. Of the common derivatives of Eugenol, it is one of the most Carnation-like.

This phenolether is used in perfume compositions as part of Carnation bases, as a fixative in spicy fragrances, as a mildly spicy note in Rose, Ylang and other florals. It is commonly used in variations of "l'Origan" type fragrances, Oriental perfumes, etc. and it blends well with Labdanum or other Ambrelike materials, with woody notes, Ionones, etc. Interesting combinations are obtained with Opopanax or Linalool or derivatives of Linalool.

This material is also used on a limited scale in flavor compositions, mainly for spice blends, Vanilla imitations, Chocolate bases, etc. The concentration used is normally about 5 to 100 ppm, as usual highest in chewing gum or certain other types of candy.

G.R.A.S. F.E.M.A. No.2476.

Prod.:

1) by Isomerization of Methyleugenol with alcoholic Potassium hydroxide.
2) by Methylation of *iso*-Eugenol with Dimethylsulfate in weak aqueous alkaline solution.

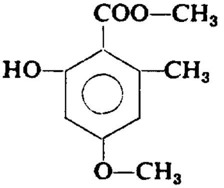
Method No. 2) is generally preferred.

4-72; 5-279; 34-1116; 77-198; 90-469; 106-257; 156-162; 160-1276;

*) The commercial material is a mixture of *trans*-Methyl-*iso*-eugenol and *cis*-Methyl-*iso*-eugenol, the latter always being the minor component (from 8 to 18% is normal). This follows the picture of *iso*-Eugenol.

## 2028: METHYL EVERNINATE

*4*-Methoxy methylorsellinate.
Methyl-*6*-hydroxy-*2*-methylanisate.
*6*-Hydroxy-*4*-methoxy-*2*-methylbenzoic acid, Methylester.
*6*-Hydroxy-*4*-methoxy-*ortho*-toluic acid, Methylester.
"Sparassol".



$C_{10}H_{12}O_4 = 196.21$

Leafy or needle-like colorless or white crystals. M.P. 68° C.

Slightly soluble in cold water and cold alcohol, soluble in hot water and hot alcohol, freely soluble in oils.

Sweet, somewhat earthy-musty odor of excellent tenacity. The earthy sweetness resembles that of Walnut and Moss, but with emphasis on the wet-mossy type. It is overall sweeter than the odor of the Ethyl-ester.

This ester, very rarely offered commercially under its proper chemical name, finds use as supporting ingredient in Oakmoss-notes, mossy bases, leather-like odors, etc. It blends beautifully with Vetiver materials and with the Coumarins, and could find extensive use if it were not for certain drawbacks.

The phenol-ether-ester is extremely sensitive to alkali, iron and mineral acids. This may explain the considerable difference in odor description appearing from reports of various observers. The sweetness is described in terms varying from "anisic" to "fungus-like" and the author believes that the odor is strongly influenced by variations in the pH of the solution in which it is studied.

Prod.:

1) by Methylesterification of Everninic acid. This esterification takes place to a measurable degree when Oakmoss is extracted with Methyl alcohol.

   Everninic acid is also a product of alkaline hydrolysis of Evernic acid which occurs naturally in Oakmoss. Evernic acid can be synthesized via Evernic aldehyde. This aldehyde is considered as an important odor factor of Oakmoss.
2) from Methylorsellinate plus Diazomethane.

7-273; 68-778; 68-788; 86-93; 90-567;

## 2029: METHYL FORMATE

Methyl methanoate.

$CH_3$—OOC—H

$C_2H_4O_2 = 60.05$

Colorless mobile liquid. Sp.Gr. 0.97.
B.P. 32° C.

25% soluble in water, miscible with alcohol, Propylene glycol, Glycerin and oils.

Very ethereal-diffusive odor of winey Chloroform-type.

The material is so volatile that it vanishes from a perfume testing blotter within seconds.

Its vapors form explosive mixtures with air, and the material presents a strong fire hazard.

Although this material is very rarely used as such in flavors, and probably never in perfumes, it will be briefly mentioned here because of its use as a "gas" in fumugating edible dried fruits (Apricots, Prunes, Pears, etc.) and Cereal. It is also used as a fumigant and larvicide for Tobacco.

The ester is occasionally used in place of Chloroform to produce a "flavor-burst" or "warm bite" in dentifrice flavors or flavors for compressed cough lozenges.

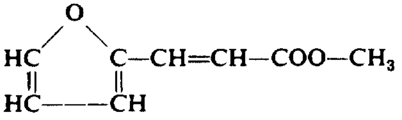
In imitation Rum flavors it may find some use as a warm-ethereal topnote, and in Raspberry flavor it can introduce a similar and quite interesting effect.

Prod.: by direct esterification of Methanol with Formic acid.

4-90; 26-604; 66-544; 77-178; 86-93; 100-678; 159-407; 160-1002; B-II-18;

## 2030: METHYL FURFURACRYLATE

Methyl-*beta*-2-furylacrylate.
(Exists in *cis*- and *trans*-isomer forms).



$C_8H_8O_3 = 152.15$

Colorless to pale straw-colored liquid or crystalline, opaque mass. M.P. 27° C.
B.P. 212° C.

Almost insoluble in water, soluble in alcohol and oils.

Balsamic-sweet, slightly fruity, tenacious odor.

This ester is used in flavor compositions, although not nearly to the same extent as the Amyl- and Allyl-esters.

It finds use as a modifier in Coffee imitation flavor, Walnut, Maple, Grape, Caramel, Butterscotch, etc.

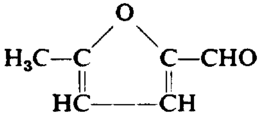
Prod.: from Furfural by Perkins' reaction to *trans*-*beta*-2-Furylacrylic acid. Methylesterification yields subject material.

69-159; 77-197; 86-93;

## 2031: alpha-METHYL FURFURAL

Methylfurfurol-(*2,5*).
*5*-Methylfurfural.
*5*-Methyl-*2*-furaldehyde.

The title name may be slightly confusing, particularly since literature has reference to a chemical named "Dimethylfuranaldehyde" (90-776), which has caused literature to use the name "*alpha*-Dimethylfurfural" in the description of what the author believes is the title material.



$C_6H_6O_2 = 110.11$

Colorless liquid. Sp.Gr. 1.10. B.P. 187° C.

3.3% soluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet-spicy, warm, and slightly caramellic odor.

Sweet-caramellic, warm taste.

This material finds some use in flavor compositions, particularly for imitation Honey, Maple, etc. and in Nut compositions, meat flavors, etc. On account of its power it is used so sparingly that the concentration in finished products is only about 0.03 to 0.15 ppm.

G.R.A.S. F.E.M.A. No.2702.

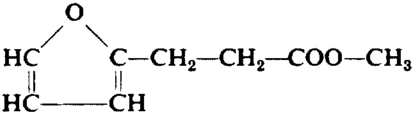
Prod.:

1) from sucrose with Hydrochloric acid, followed by treatment with Stannous chloride.
2) from various Methylpentoses by distillation with acid.

7-136; 26-604; 69-154; 86-93; 160-1006; B-XVII-289; 90-775; 157-472;

## 2032: METHYL FURFURHYDRACRYLATE

Methyl-*2*-furanpropionate.
Methyl furyl propionate.



$C_8H_{10}O_3 = 154.17$

Pale yellowish liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Fruity-woody odor, but rather sharp-green when undiluted. Moderate to poor tenacity.

Dry-fruity and relatively pleasant taste in concentrations below 50 ppm. (The Ethylester is permitted in food flavors in the U.S.A.).

This ester finds some use in flavor compositions (outside of the U.S.A.) particularly Blackcurrant, Pineapple, Rum, etc. or in fruit complexes.

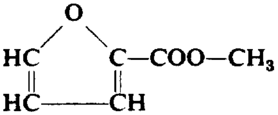
The author has no record of its use in perfume compositions.

Prod.: from Furfural via Furfurylacrylic acid to Furan propionic acid, which is esterified with Methanol.

(See also: Ethyl furfurhydracrylate and *iso*-Butyl furfur hydracrylate).

## 2033: METHYL FUROATE

Methyl-*2*-furoate.
Methyl pyromucate.
Furan-*alpha*-carboxylic acid, Methylester.



$C_6H_6O_3 = 126.11$

Colorless liquid. (It turns yellow or dark when exposed to daylight).

Sp.Gr. 1.18. B.P. 181° C.

Very slightly soluble in water, soluble in alcohol and oils.

Berry-like fruity, winey and rather heavy odor of moderate to poor tenacity. Some observers find a nauseating or fungus-like Tobacco odor.

Sweet-tart, heavy, fruity taste, often compared to Ethyl lactate, Ethyl acetate and Ethyl benzoate.

This ester find limited use in flavor compositions, e. g. in trace amounts in meat flavors. The concentration equals about 0.1 to 1 ppm in the finished product.

The author is not aware of any use in perfumery of this ester.

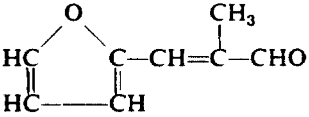
G.R.A.S. F.E.M.A. No.2703.

Prod.: from Furfural via oxidation or Canizzaro's reaction to *2*-Furoic acid which is esterified to subject material.

26-604; 31-127; 7-273; 69-157; 86-93; 160-1008; B-XVIII-274;

## 2034: alpha-**METHYL**-beta-**FURYL ACROLEIN**

*alpha*-Methyl-*beta*-*2*-furylacraldehyde.
*2*-Methyl-*3*-furylacrolein.
*alpha*-Methyl furanacrolein.
*alpha*-Methyl furfuracrolein.
*2*-Methyl-*3*-(*2*-furyl)-propenal.



$C_8H_8O_2 = 136.15$

Pale yellowish liquid. Sp.Gr. 1.10.
B.P. 225° C.

Very slightly soluble in water, soluble in alcohol and oils.

Mild, but warm, Cinnamon-like odor of moderate to poor tenacity. Compared to Furanacrolein (crystalline material) it is perhaps milder, but also less woody, softer and sweeter.

This aldehyde finds use in flavor compositions, not only in spicy types, but also in Nut compositions, Chocolate, fruit, etc. and occasionally in Maple-Walnut.

The concentration used is about 0.5 to 1 ppm in the finished product.

The aldehyde is, to the author's knowledge, not used in perfumery, although it could find interest as a variant of the equivalent aldehyde: *alpha*-Methylcinnamic aldehyde.

This material shows less tendency to discoloration than the crystalline Furanacrolein.

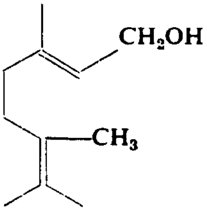
G.R.A.S. F.E.M.A. No.2704.

Prod.: by condensation of Furfural and Propionaldehyde.

31-40; 69-154; 93-150;

## 2035: METHYL GERANIOL

*3,6,7*-Trimethyl-*2,6*-octadienol.
*3*-Methyl geraniol.
The commercial material is of poorly specified Nature and should not be confused with:
Methyl geranyl ether (see monograph) also called Geranyl methylether.
Ethyl geraniol (see monograph) which is an isomer.



$C_{11}H_{20}O = 168.28$

Colorless or very pale straw-colored oily liquid. B.P. 216° C.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-rosy odor, sweeter and slightly more citrusy than Geraniol, moderate to poor tenacity.

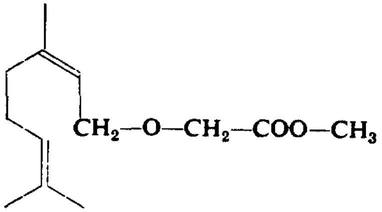
This rare item has been suggested for use in perfume compositions as a modifier for the conventional "rose alcohols", but it is still too expensive to be used in similar proportions or for low-cost fragrances. It blends very well with Citronellol and its esters, with Citrus oils, Bergamot in particular, and with Hydroxycitronellal.

Prod.: from Geraniol with Dimethylsulfate and Pyridine by heating in Diethylene glycol at 200-210° C.

4-90; 86-93; 163-221; 163-360;

## 2036: METHYL GERANOXYACETATE

Methyl geranyloxyacetate.
Geranoxyacetic acid, Methylester.



$C_{13}H_{22}O_3 = 226.32$

Colorless oily liquid. B.P. 253° C.

Insoluble in water, soluble in alcohol and oils.

Weak, but delicately rosy and tenacious odor. The mildness or weakness of this odor is often translated as "musky", but the true odor of this and many similar odorants are only understood when the materials are used along with more volatile components in a composition.

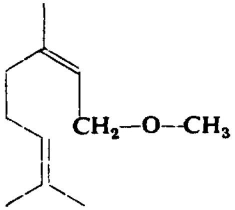
The oxyester finds some use in perfume formulations, mainly for light-green and delicate florals, Peony, Muguet, etc.

See also: Ethyl geranoxyacetate.

31-159;

## 2037: METHYL GERANYL ETHER

Geranyl methyl ether.
Commercial grades are not chemically pure or well-defined. Most of these products contain substantial amounts of Linalyl methylether, Linalool and related materials.
See also: Ethyl geranyl ether.



$C_{11}H_{20}O = 168.28$

Colorless oily liquid. B.P. 210° C.
Sp.Gr. 0.84.

Almost insoluble in water, soluble in alcohol and oils.

Green-leafy, slightly "weedy", oily-rosy, but overall refreshing "outdoorish" odor of moderate to poor tenacity.

It bears some resemblance to the odor of Citral dimethylacetal.

This ether has been suggested for use in perfume formulations, and could probably be useful in topnote compositions with Citrus oils, foliage-green notes, Lavender-Lavandin, and in certain types of floral fragrance, e. g. Muguet, Narcisse, etc.

Variations in odor of material from different suppliers is one factor contributing to great reluctance on the part of the perfumers to use this material widely.

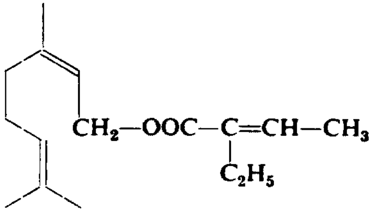
Prod.: (several methods), e. g. from Geranyl chloride plus Sodium methoxide in Methanol.

Also by isomerization of Linalool under Methyl-alcoholic conditions.

4-56; 86-55;

## 2038: METHYL GERANYL TIGLATE

Geranyl methyl tiglate (commercial name).
Geranyl-*alpha*-ethylcrotonate (*cis*- and *trans*-forms).
Geranyl methylethyl acrylate.



$C_{16}H_{26}O_2$ = 250.38

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-floral, slightly fruity odor of Bergamot-Geranium-Rose type- and fair to good tenacity.

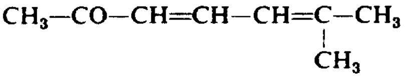
This rare ester is occasionally used in perfume compositions as a modifier in light floral bases, Muguet, Lily, Rose, Peony, Freesia, etc. and as a novel note in Chypre or Citrus colognes. It is not regularly available, and the author understands that the original manufacturer has discontinued production of this item.

Prod.: from Geraniol and *alpha*-Ethylcrotonic acid. The acid is obtained from Bromdiethylbutyric acid by depriving that material of Hydrogen bromide.

4-56;

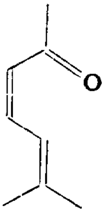
## 2039: 2-METHYLHEPTADIEN-(2,4)-ONE-6

6-Methylheptadien-3,5-one-2.
Methylheptadienone.



$$CH_3{-}CO{-}CH{=}CH{-}CH{=}\underset{\displaystyle CH_3}{\underset{|}{C}}{-}CH_3$$

or:



$C_8H_{12}O$ = 124.18

Pale yellowish or almost colorless oily liquid.
B.P. 190° C. Sp.Gr. 0.90.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, yet warm-spicy, Cinnamon-like and simultaneously Coconut-like slightly fruity odor with sweet, oily-Nut-like undertones. Moderate to poor tenacity.

This unsaturated ketone is interesting not only by its difference from Methylheptenone, but also in having a distinct Cinnamon-character, usually connected with aldehydes of cyclic or heterocyclic type, or occasionally lower alifatic ketones. Coconut character is found frequently in C-9 ketones, esters, lactones, etc. but not often in C-8.

The subject material has only been commercially available on a large scale since the early 1960's, and is not yet widely used. It is quite possible that the reluctance on the part of the perfumers to use unsaturated or polyunsaturated ketones is cosmetic fragrances can work against this material. However, there is no published evidence that the material can not be used safely, and since it is so powerful, it may well be compared to many, perhaps hazardous, materials, permissible in perfumes at low concentration.

It has very interesting effect as a "natural" topnote in artificial Lavandin, a fact which could be studied along with experiments with Benzylidene acetone and Cinnamylidene acetone in same composition. For novel spicy effects and for unusual power in Oriental fragrance types, the subject ketone has certainly many possibilities.

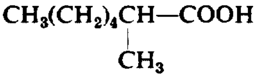
Since the ketone is not included in the Federal Register as G.R.A.S. it would be wise to have its pharmacological effects investigated before it is used in flavors beyond laboratory experiments. It could undoubtedly find good use in Cinnamon flavors, spice blends, Nut compositions, Tutti-frutti flavors, etc.

Prod.: *2*-Methylbuten-*2*-al-*4* is reacted with Acetone in presence of Sodium ethylate or hydroxide. Various isomers are produced along with subject ketone.

(Sample: Hoffmann-laRoche, Inc.).
89-189;

## 2040: 2-METHYL HEPTANOIC ACID

Hexane-*2*-carboxylic acid (British nomenclature).
*iso*-Caprylic acid.
*iso*-Octanoic acid.
Methyl amyl acetic acid.
*2*-Methyl oenanthic acid.



$$CH_3(CH_2)_4\underset{CH_3}{\underset{|}{CH}}-COOH$$

$$C_8H_{16}O_2 = 144.26$$

Colorless oily liquid, solidifying in the cold to a white or colorless crystalline, leafy-scaly mass of translucent crystals. M.P. 15° C. B.P. 220° C.

Almost insoluble in water, soluble in alcohol and oils.

Fatty-oily, rather unpleasant sour odor, but not sweat-like, rancid as the normal Caprylic acid.

Sour-fruity, somewhat oily-nutty taste.

This acid is occasionally used in flavor compositions, where a sour-fruity note is desirable as part of the fruity flavor complex, e. g. Apple, Berry, Apricot, etc. and in Coconut flavors.

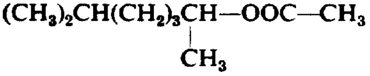
The concentration is normally low, about 1 to 10 ppm in the finished product.

Prod.: by oxidation of *alpha-n*-Amylpropionic aldehyde.

G.R.A.S. F.E.M.A. No.2706.

## 2041: 2-METHYLHEPTANOL-6-ACETATE

*6*-Methylheptanyl-*2*-acetate.
"*iso*-Octylacetate".
Methyl-*iso*-hexylcarbinylacetate.
"Fructurol".
*iso*-Propyl-*secondary*-Amylacetate.



$$(CH_3)_2CH(CH_2)_3\underset{CH_3}{\underset{|}{CH}}-OOC-CH_3$$

$$C_{10}H_{20}O_2 = 172.27$$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Intensely fruity, sweet and slightly oily odor of moderate tenacity. The odor is less herbaceous, also less floral than that of the normal Octyl acetate.

Sweet-fruity, quite powerful taste of Strawberry-Peach complex type.

This ester is used in perfume compositions as part of fruity complexes, bases or topnotes. It introduces freshness to Ethyl methyl phenyl glycidate or Undecanolide, and its fruity note is rather nondescript, i. e. it will emphasize almost any other type of fruity note.

The material is also used in flavor compositions, although not in all countries. It is particularly suitable for Banana, Strawberry, Mango, Peach, Melon, etc. and could be used as a modifier in "Tutti-frutti" complexes.

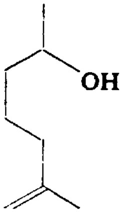
Prod.: by direct esterification under azeotropic conditions.

(See also Methyl-*iso*-hexylcarbinol).
No. 2058.

86-93;

## 2042: METHYL HEPTENOL

2-Methyl-*n*-hepten-*1*-ol-*6*.



$C_8H_{16}O = 128.22$

Colorless oily liquid. B.P. 180° C.
Sp.Gr. 0.85.

Very slightly soluble in water, soluble in alcohol and oils.

Oily-green, herbaceous-citrusy odor with resemblance to Coriander and unripe berries. Its freshness resembles that of Citraldimethylacetal, the green notes resemble those of Blackcurrant.

This alcohol, not nearly as penetrating in odor as the ketone (see following monograph), finds some use in perfume compositions as a minor part of topnote bases for Citrus colognes, Oriental bases, Rose modifications, etc.

Prod.:

1) by reduction or catalytic hydrogenation of Methylheptenone.
2) from Geranonitrile by boiling it with alcoholic Potassium hydroxide.

4-90; 7-77; 7-255; 7-273; 35-60; 35-402; 86-93; 87-484; 89-186; 114-14;

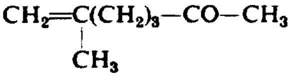
## 2043: 2-METHYLHEPTENONE

Methyl hexenyl ketone.
*2*-Methyl-*2*-hepten-*6*-one.
Commercial (unpurified) product contains usually about 20% *2*-Methyl-*1*-hepten-*6*-one*).

Subject material:

$(CH_3)_2C{=}CH{-}CH_2{-}CH_2{-}CO{-}CH_3$

and the impurity*):



$$CH_2{=}\underset{\displaystyle CH_3}{\underset{|}{C}}(CH_2)_3{-}CO{-}CH_3$$

$C_8H_{14}O = 126.20$

Colorless mobile oily liquid. Sp.Gr. 0.86.
B.P. 174° C.

Insoluble in water, soluble in alcohol and oils.

Oily-green, pungent-herbaceous, grassy and diffusive odor with fresh and green-fruity notes and moderate to poor tenacity.

In extreme dilution (below 5 ppm) it has a fruity, green-Banana-like or unripe Berry-like taste. Higher dilutions produce harsh and pungent notes.

This ketone, available at a very low price in a commercial (impure) grade as a by-product from processing of Citronella and Lemongrass oils or in the manufacture of Ionones, finds quite extensive use although mostly at very low concentrations in soap perfumes, detergent or masking odors, perfumes for household or "heavy-duty" purposes, in insecticide sprays or other products calling for powerful masking odors.

It is also used sparingly in Citrus colognes, Sweet Pea, Oriental bases, Rose variations, New Mown Hay, and in general as part of powerful green-floral topnote complexes. It is generally agreed that the above mentioned impurity is largely responsible for the "grassy" odor in the commercial product. Pure Methylheptenone is available and has, indeed, a less fatty-grassy odor.

The ketone is used in flavor compositions in minute traces, primarily in imitation Apple, Banana, Citrus, Date, Blackcurrant, Mulberry, Raspberry, Melon, Peach, Pear, Pineapple, etc.

The concentration is normally about 1 to 2 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2707.

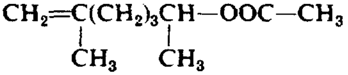
Prod.:

1) from fractions of Citronella oil or Lemongrass oil.
2) by oxidation of Geraniol or related materials (Citral, etc.).
3) from Acetoacetic ester plus Methylbuten-*3*-ol-*2* with Aluminum alcoholate in Carroll's reaction, followed by pyrolysis of the resulting ester.
4) numerous other methods.

26-606; 31-19; 35-60; 4-90; 66-533; 77-211; 86-93; 89-183; 106-249; B-I-741;

## 2044: METHYL HEPTENYL ACETATE

*2*-Octenyl acetate.



$$CH_2=\underset{\begin{array}{c}|\\CH_3\end{array}}{C}(CH_2)_3\underset{\begin{array}{c}|\\CH_3\end{array}}{C}H-OOC-CH_3$$

$C_{10}H_{18}O_2 = 170.25$

(For "acyclic monoterpene structure" – see Methyl heptenol).

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Oily-green, almost earthy or slightly musty-fungoid odor of moderate to poor tenacity.

This ester is occasionally used in perfume compositions as part of the green theme in Reseda or other earthy-green floral complexes.

Its peculiar odor puts a rather strict limit to its use, and it is not nearly as versatile as its isomer, Amyl vinyl carbinyl acetate (*3*-Octenyl acetate).

Prod.: by direct esterification of Methylheptenol with Acetic acid under azeotropic conditions.

35-402; 113-15;

## 2045: METHYL HEPTIN CARBONATE

Methyl-*n*-hept-*1*-yne-*1*-carboxylate.
"Folione" (Givaudan).
Methyl-*2*-octynoate.
"Vert de Violette" (name also used for higher homologues).
"M.H.C."

$CH_3(CH_2)_4C{\equiv}C-OOC-CH_3$

$C_9H_{14}O_2 = 154.21$

Colorless or very pale straw-colored liquid. Sp.Gr. 0.93. B.P. 217° C.

Almost insoluble in water, soluble in alcohol and oils, almost insoluble in Propylene glycol and Glycerin.

Very powerful, penetrating vegetable-green foliage type odor of moderate to poor tenacity.

This acetylenic ester was once the ideal material for Violet-foliage and fresh-green vegetable odors, Cucumber odor, etc. The explosive rate of development of new aromatic chemicals for perfumes during the past 20 years has brought particularly many "green" materials on the market, including practically all of those identified in natural materials. Very few acetylenic esters have been identified in natural products, and the subject material is not one of them.

Its limited stability and its reputation of being a possible skin-irritant are factors contributing to the declining use of this ester. However, it still finds use in many perfume compositions, not only in Violet and Cucumber. Its use with the conventional Ionones and Eugenols and perhaps Cyclamenaldehyde can be modified with even more interesting effect when the Ionones are replaced with special Methyl ionones, the Eugenols are limited to substituted *iso*-Eugenols, and Cyclamal is replaced by Lilial or the like.

The appearance of fatty-waxy notes is a common and well-known feature when this ester is overdosed in a fragrance or a base. Its tenacity can be improved by proper blending, e. g. as above suggested.

The subject material finds some use in flavor compositions, mainly for Cucumber, Berry-complexes, Fruit blends, Peach imitation, Liqueur flavorings, various "floral" flavors, "muscatel" flavors, etc.

The concentration is normally about 0.1 to 2 ppm, but in chewing gum it may reach 10 to 20 ppm.

G.R.A.S. F.E.M.A. No.2729.

Prod.: from Heptyne or from *n*-Heptanal via Heptylidene chloride and by reduction to Heptyne which is carboxylated to the acid from which the ester is prepared.

4-90; 5-241; 31-123; 77-188; 85-86; 85-155; 85-157; 106-250; 103-295; 156-7;

## 2046: METHYL HEPTOATE

Methyl heptanoate.
Methyl heptylate.

NOTE: The name "Methyl oenanthate" is sometimes applied to a material which may be the heptanoate. For nomenclature see Ethyl heptanoate and Ethyl oenanthate.

$CH_3—OOC—C_6H_{13}$

$C_8H_{16}O_2 = 144.22$

Colorless mobile liquid. Sp.Gr. 0.88. B.P. 174° C.

Insoluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Fruity-green, slightly waxy-berry-like odor of poor tenacity.

Sweet-oily fruity, fresh, somewhat green-tart taste.

This ester finds use in flavor compositions mainly for Gooseberry, Apple, Peach, Apricot, Pear, Pineapple, Grape and various berry-complexes.

The concentration is mere traces, about 0.5 to 1 ppm in the finished product.

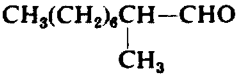
G.R.A.S. F.E.M.A. No.2705.

Prod.: by direct esterification of *n*-Heptanoic acid with Methanol under azeotropic conditions.

4-90; 7-274; 26-606; 35-59; 86-93; 160-968; B-II-339;

## 2047: METHYL HEPTYL ACETALDEHYDE

An *iso*-Decylaldehyde.
*2*-Methylnonanal.



$CH_3(CH_2)_6CH(CH_3)—CHO$

$C_{10}H_{20}O = 156.27$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful and diffusive woody-green, also slightly citrusy odor of moderate to poor tenacity.

This aldehyde is very rarely offered under its proper chemical name, but it finds use as a "captive" chemical inside many perfume houses with chemical manufacturing facilities.

Its odor beauty and versatility are far from comparable to those of Methyl nonyl acetaldehyde, and although it is true that several branched-chain alifatic aldehydes have proved to be of considerable interest, this material does not seem to be one of them. Its odor is rather dry and it does not blend easily with the conventional aldehydes.

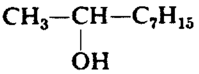
Prod.: by Darzen's type synthesis by condensation of Methylheptylketone with Ethyl monochloroacetate in presence of Sodium ethanoate, followed by hydrolysis to the acid and heating under vacuum to produce the aldehyde.

Also from *alpha*-Heptyl acrolein by hydrogenation.

4-90; 35-60; 103-188;

## 2048: METHYL HEPTYL CARBINOL

*secondary-n*-Nonanol.
*2*-Nonanol.
*n*-Nonanol-*2*.



$$CH_3-\underset{\displaystyle OH}{\underset{|}{CH}}-C_7H_{15}$$

$C_9H_{20}O = 144.26$

Colorless liquid. Sp.Gr. 0.82. B.P. 194° C.

Insoluble in water, soluble in alcohol and oils.

Powerful fruity-green, slightly oily-floral odor of moderate to poor tenacity. This is indeed a material that receives quite a variation of odor descriptions from different observers.

It finds some use in perfume compositions, mainly as part of the topnote complex in green-floral bases, such as Gardenia or Carnation, or it may be a trace component in spice compositions where it introduces a pleasant freshness, particularly if there is a citrus note present. It gives a similar effect in Lavender or other herbaceous compositions.

The alcohol finds limited use in flavor compositions as a trace ingredient in Coconut flavors or in various spice blends.

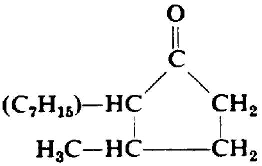
Prod.:

1) by hydrogenation of Methyl heptyl ketone.
2) by Grignard type synthesis from Heptyl magnesium bromide plus Acetaldehyde.

26-640; 28-530; 77-172; 160-1126; B-I-423;

## 2049: 3-METHYL-2-n-HEPTYL CYCLOPENTAN-1-ONE

*2-n*-Heptyl-*3*-methylcyclopentan-*1*-one.
"Cyclamon". (Cyclamone).
Homo-dihydro-*iso*-jasmone.



$C_{13}H_{24}O = 196.34$

Colorless or very pale straw-colored oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, fruity-herbaceous and sweet-floral odor of good tenacity. It has a great deal in common with certain types of *iso*-Jasmone, but is not quite as pungent or powerful.

This ketone, usually offered under various trade names, is used in floral compositions as a diffusive and powerful factor, supporting the conventional floralizers, or introducing a novel type of fruity floral note, perceptible with the topnote and, if the fixation is properly created, continuing into the terminal notes of the fragrance.

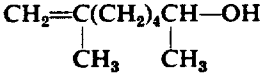
It is perhaps less Jasmin-like, more Sweet-Pea or Lindenblossom like, and it blends well with Cyclamen aldehyde, Heliotropine, Hydroxycitronellal, etc,

Prod.: by hydrogenation of the *2*-unsaturated ketone which is prepared from *2,5*-Tridecandione, a *gamma*-Diketone.

5-153; see also: 156-223;

## 2050: METHYL HEPTYLENE CARBINOL

"*iso*-Nonylene alcohol".
*2*-Nonenol-*7*.
Do not confuse with: *n*-Nonen-*2*-ol-*1*.
(= Hexyl allyl alcohol).



$CH_2{=}\underset{CH_3}{C}(CH_2)_4\underset{CH_3}{CH}{-}OH$

$C_9H_{18}O = 142.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, fatty-fruity, oily and slightly herbaceous odor. Overall not very pleasant. Some observers find a green-earthy or fungoid note.

This unsaturated alcohol has found a little use in perfume compositions mainly for reinforcing Lavender notes for soap use and for other purposes where power is particularly called for.

7-274;

## 2051: METHYL HEPTYL ETHER

Heptyl methyl ether.

$CH_3{-}O{-}C_7H_{15}$

$C_8H_{18}O = 130.23$

Colorless oily liquid. B.P. 151° C.
Sp.Gr. 0.79.

Insoluble in water, soluble in alcohol and oils.

Tart-green, fresh-foliage-like odor, resembling aldehydic-green odors. Moderate to poor tenacity. The odor has been described as resembling that of freshly crushed berries of mountain ash.

This ether has found a little use in perfumery as a modifier in fresh-green notes, particularly in topnote compositions for herbaceous or green-floral fragrances types. It blends favourably with Lavender, Bayberry-notes, Fougeres, etc. and it can be blended into Apple-type bases or compositions. It has the advantage of being quite powerful and stable in soap or powders, but it requires solid fixation.

Prod.: from *n*-Heptylchloride plus Sodium methoxide in Methanol solution.

4-90; 35-60;

## 2052: METHYL HEPTYL KETONE

Nonan-*2*-one.
*2*-Nonanone.

$CH_3{-}CO{-}C_7H_{15}$

$C_9H_{18}O = 142.24$

Colorless oily liquid. Sp.Gr. 0.83.

B.P. 194° C. Solidifies in the cold, melts at minus 15° C.

Insoluble in water, soluble in alcohol and oils.

Fruity-floral, slightly fatty and herbaceous odor of moderate to poor tenacity.

This ketone finds some use in perfume compositions as a powerful ingredient in Lavender compositions, in Citrus cologne types and in variations of New Mown Hay, etc.

Its proper odor is not exactly agreeable, and it serves mainly the purpose of increasing the power and diffusion of the fragrance in which it is incorporated.

It finds also some use in flavor compositions, e. g. in imitation Rose and Tea, in fruit complexes or various berry compositions. The concentration is usually very low, about 0.1 to 0.5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2785.

Prod.:

1) by Grignard type synthesis from Octyl magnesium bromide with Ethyl formate or *ortho*-Formic ester.
2) by oxidation of *secondary*-Nonylalcohol.

4-90; 31-80; 35-60; 66-516; 86-93; 160-1126;

## 2053: METHYL-2-HEXENOATE

Methyl-*beta*-propylacrylate.
Methyl-*alpha-beta*-hexenoate.
Do not confuse with: Methyl hexadienoate, which is Methyl sorbate.

$CH_3—CH_2—CH_2—CH{=}CH—COO—CH_3$

$C_7H_{12}O_2 = 128.17$

Colorless mobile liquid. B.P. 169° C.

Very slightly soluble in water, soluble in alcohol and oils.

Green-musty, earthy-sweet and fruity odor of moderate to poor tenacity.

This ester is used in flavor compositions for the type of fruit flavor demanding a rather sharp and green fruity topnote, such as Pineapple, Strawberry, etc. and in various fruit complexes. It is quite powerful, and the concentration used is normally equivalent to only 0.05 to 0.1 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2709.

Prod.: by direct esterification. The acid is obtained from reacting Butyraldehyde with Malonic acid. A certain amount of *3*-Hexenoic acid is formed, but it can be rearranged to the *2*-Hexenoic acid.

Esters of the *2*-Hexenoic acid are present in Mentha arvensis oil.

(See also: 90-121).

## 2054: METHYL HEXENYL ETHER

*1*-Hexen-*6*-yl methylether.
*omega*-Hexenol methylether.

$CH_3—O—(CH_2)_4—CH{=}CH_2$

$C_7H_{14}O = 114.19$

Colorless mobile liquid. B.P. 147° C.

Practically insoluble in water, soluble in alcohol and oils.

Sharp-green, very diffusive odor of very poor tenacity.

This ether, very rarely offered commercially, has probably little if any value in perfumery. It was developed along with many related materials, Hexenols, Hexenylesters, etc. However, it does not lend any particularly pleasant or natural-green notes to a fragrance, and it is not as chemically accessible as the conventional Hexenol derivatives.

The author feels that it is – or will soon be – an obsolete item.

## 2055: METHYL HEXIN CARBONATE

Methyl-*2*-heptynoate.

$CH_3(CH_2)_3{\equiv}C—COO—CH_3$

$C_8H_{12}O_2 = 140.18$

Colorless liquid. B.P. 190° C.

Insoluble in water, soluble in alcohol and oils.

Powerful and very diffusive, foliage-green, somewhat pungent, but also sweet odor of moderate to poor tenacity.

Its greenness is generally considered more pleasant and less fatty-oily than that of the more common Methyl heptin carbonate.

The subject material is rarely offered as such, but forms part of several "specialties", sold under trade names. The specialties often contain higher homologues of subject material.

It finds some use in perfumery, where it may constitute a minor part of green topnotes often in combination with fruity notes. Its main purpose is that of supplying the necessary foliage notes in Violet, Narcisse, Cassie and similar floral bases, occasionally also in imitation Cucumber odor.

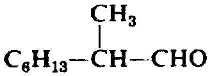
Newer and more true-to-Nature chemicals have substituted the acetylenic esters in many cases, and it is not likely that these esters will live far out in the future of perfume chemistry.

Prod.: (many methods) e. g. from Hexaldehyde via Hexyne to the carboxylic acid, which is subsequently esterified. Also from Methyl-*n*-butylketone via *n*-Hex-*1*-yne.

5-245;

## 2056: METHYL HEXYL ACETALDEHYDE

"*iso*-Nonylaldehyde" (a somewhat ambiguous name).
*2*-Methyl octanal.
"7-Methyl nonyl aldehyde" (misleading name)



$$C_6H_{13}-\underset{}{\overset{CH_3}{\overset{|}{C}}}H-CHO$$

$C_9H_{18}O = 142.24$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Delicately floral, fresh-"aldehydic" odor, much less fatty than Nonanal, more rosy, Lily-like. Moderate tenacity.

This aldehyde, more conspicuous by its absence from so many perfume laboratories, is used with excellent effect by the few who really enjoy experimenting with unconventional materials.

In effect more versatile than Methyl nonyl acetaldehyde, it creates floral-diffusive topnotes in a Lily or Muguet, freshness in Mimosa or Rose, gives clean and airy topnotes to Citrus fragrances, etc.

It finds some use in flavor compositions, mainly in Citrus types where it may partly or wholly substitute the conventional Nonanal. Concentration used is about 1 to 2 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2727.

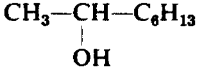
Prod.:

1) from Hexanal and Propionic aldehyde.
2) by Darzen's synthesis: Methyl hexylketone plus Ethyl chloroacetate and Sodium ethylate. Hydrolysis of the ester resulting, and heating under vacuum of the acid obtained from the hydrolysis.

7-275; 8-163; 159-408; 31-49;

## 2057: METHYL HEXYL CARBINOL

Octanol-*2*.
*secondary*-Octylalcohol.
*secondary, inactive* Caprylalcohol.
*2*-Octanol.
*secondary*-Alcohol C-8.
Hexyl methyl carbinol.



$$CH_3-\underset{OH}{\underset{|}{C}}H-C_6H_{13}$$

$C_8H_{18}O = 130.23$

Colorless oily liquid. B.P. 179° C.
Sp.Gr. 0.82.

0.1% soluble in water, soluble in alcohol, Propylene glycol and oils.

Odor descriptions reported or published on this chemical vary enormously. The main reason must be sought in the fact that the material is offered in a "technical" grade, very inexpensive, from several petrochemical companies, while certain perfume chemical manufacturers may offer material of their own production. The two types of product are quite different in chemical purity and composition.

The relatively pure chemical has a pleasant, mild-green, floral-leafy and somewhat musty odor, almost reminiscent of dry tea leaves. Its woody-herbaceous notes remind of Coriander with a citrusy freshness. The odor is distinctly less fatty than that of *n*-Octanol-*1*.

The "technical" grade shows generally the musty note as the chief note, with little or no citrusy or floral or mild odors.

The taste (of the relatively pure material) is slightly musty, green and remotely fruity, berry-like. It shows bitterness in concentrations above 10 ppm.

This secondary alcohol is used extensively in masking odors ("technical grade") or other fragrances for industrial or "heavy-duty" household purposes. The purer grade material is used in herbaceous perfumes, Fougères, Chypres, etc. to a limited degree.

Trace amounts are used in imitation Blackcurrant flavor or certain types of Nut flavor, particularly Walnut (musty note), and in Coriander condiments.

Concentrations range from 0.5 to 5 ppm in the finished products.

G.R.A.S. F.E.M.A. No.2801.

Prod.:

1) by heating and distilling Sodium ricinoleate in presence of Sodium hydroxide.
2) by hydrogenation of Methyl hexyl ketone.

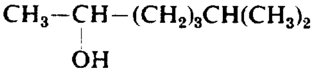
4-90; 5-69; 29-476; 35-400/401/402; 86-106; 100-742; 160-1130; 163-58; 163-228;

## 2058: METHYL-iso-HEXYL CARBINOL

"*iso*-Octylalcohol" (somewhat ambiguous name).

*6*-Methylheptanol-*2*.

*2*-Methylheptanol-*6*.



$$CH_3-\underset{\displaystyle OH}{\underset{|}{C}H}-(CH_2)_3CH(CH_3)_2$$

$$C_8H_{18}O = 130.23$$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-green, slightly floral-dry odor of moderate to poor tenacity.

This alcohol is not widely used in perfumery, but its acetate is known under the trade name of "Fructurol", see monograph: *2*-Methylheptanol-*6*-acetate.

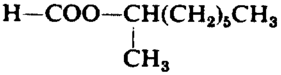
Prod.: by complete hydrogenation of Methylheptenone (*6*-Methyl-*5*-hepten-*2*-one).

## 2059: alpha-METHYL-n-HEXYL CARBINYL FORMATE

Methyl hexyl carbinyl formate.

Octanyl-*2*-formate.

*iso*-Caprylic formate.



$$H-COO-\underset{\displaystyle CH_3}{\underset{|}{C}H}(CH_2)_5CH_3$$

$$C_9H_{18}O_2 = 158.24$$

Colorless liquid. Sp.Gr. 0.87. B.P. 187° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Warm-herbaceous, slightly green-spicy and fruity-rosy, sweet odor, remotely resembling notes of Opopanax.

This ester finds a little use in perfume compositions as part of "Oriental" fragrance complexes or as a trace component in variations of Chypre, etc. It blends very well with Labdanum and Rose notes, and gives interesting effect in Lavender or Clary Sage. It is also used in flavor compositions for fruit bouquets.

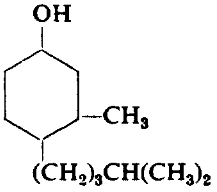
Prod.: from *d*-Octanol-*2* with anhydrous formic acid and Zinc chloride.

163-58;

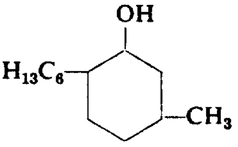
**Note**: Literature includes: Ethyl-*n*-amyl carbinylformate which is *3*-Octanyl formate, an isomer of the title material.

## 2060: 3-METHYL-4-iso-HEXYL CYCLOHEXANOL (A), and: 3-METHYL-6-HEXYL CYCLOHEXANOL (B)

(A): *4*-Hydroxy-*6*-methyl-*1*-*iso*-hexylcyclohexane.
(B): *2*-Hydroxy-*4*-methyl-*1*-hexylcyclohexane.



(A)



(B)

$C_{13}H_{26}O = 198.35$

Colorless liquids.

Insoluble in water, soluble in alcohol and oils.

These two alcohols are briefly mentioned in this work as examples of di-alkylsubstituted Cyclohexanols of possible interest to the perfumer.

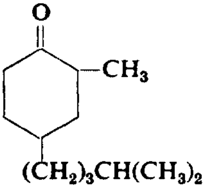
Three Methyl hexyl cyclohexanones are mentioned in this book (see monographs), but it is fair to say that none of these materials have reached any "volume" level, let alone reached the shelves in the majority of all perfume laboratories. Research has brought us an enormous number of Cyclohexanol derivatives, and a few have become everyday items.

The above materials do not distinguish themselves by unusual odor type or any other dramatic advantage. They carry the almost conventional "camphoraceous-woody" note, although material (B) can be classified as primarily floral with an Ionone-like woody note. They have power and they are relatively inexpensive, but they must be available in a stable odor quality and definite chemical quality before they can hope for a firm place on the perfumer's shelf.

Prod.: from the corresponding ketones by hydrogenation. Three isomer ketones are mentioned in this work. (See next).

4-109;

## 2061: METHYL-2-iso-HEXYL-4-CYCLOHEXANONE-1



$C_{13}H_{24}O = 196.34$

White crystalline material. M.P. 39° C.

Warm, mild, but tenacious musky-orrislike odor. The camphoraceous notes so often encountered in Cyclohexanone derivatives, are pleasantly subdued and generally accepted as Orris-like rather than Camphor-like.

More than thirty years ago, perfume chemistry research had the alkyl-substituted cyclohexanones, etc. under investigation, and a few successful materials are still appearing on the market from time to time.

The three isomers described here have all reached the commercial marketing level, but it is too soon to state that they have established a successful position as standard perfume chemicals.

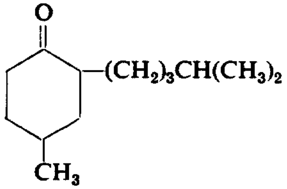
The cost of the material is often an overwhelmingly important factor when it comes to powerful chemical odorants intended for volume use. If they can not find a place in soap or detergent perfumes or similar large-volume outlet, chances are that they will never be produced at a really low cost, because volume is a prerequisite for sufficiently low cost. In other words, "the evil circle" of perfume chemicals, such as one can see with the essential oils: someone has to pay for the start of the material, and it is not always the producer.

The subject ketone may find use in novel and masculine type soap fragrances, room sprays, etc. should it ever become commercially available at a sufficiently attractive price.

Prod.: by hydrogenation of *para-iso*-Hexyl-*ortho*-cresol to the secondary alcohol, which is subsequently oxidized to the ketone. 2 isomers are produced similarly, and separation of the isomers depends partly upon the composition of the original Cresol.

(Parfumerie, Cosmetique, Savons, August 1965).

## 2062: METHYL-4-iso-HEXYL-2-CYCLOHEXANONE-1



$C_{13}H_{24}O = 196.34$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Dry-woody, orrisy and tenacious odor.

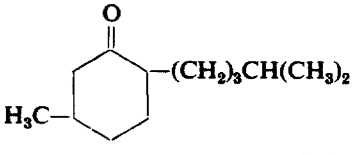
This is the odortype most frequently met with in the study of derivatives of Cyclohexanone, and the perfumer may sometimes feel that he is inondated with this type of new chemical odorants.

It could find use in soap perfumes as a modifier/blender for Ionones and Methylionones, but its dry character puts a rather low limit to the practical concentration of this ketone in a composition.

See comments under Methyl-*2-iso*-hexyl-*4*-cyclohexanone (previous monograph).

Parfumerie, Cosmetiques, Savons, August 1965.

## 2063: METHYL-5-iso-HEXYL-2-CYCLOHEXANONE-1



$C_{13}H_{24}O = 196.34$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils. Almost insoluble in Propylene glycol.

Soft, creamy-floral and sweet odor of moderate to good tenacity. The odor bears an interesting similarity to that of *para-tertiary*-Butylcyclohexylacetate, a very common fragrance chemical.

The odor of this isomer is, in the author's opinion, most likely to strike success, although this odor is already represented by several derivatives of Cyclohexanol, since long ago on the market.

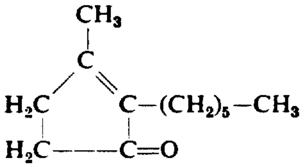
This ketone is quite versatile. It falls smoothly into the Ionones and Methylionones, it blends well with the "rose alcohols" and Amylcinnamic aldehyde, it suports Ylang-Ylang notes and forms a good background for Fougère in soap.

See also comments under Methyl-*2-iso*-hexyl-*4*-cyclohexanone (earlier monograph).

Parfumerie, Cosmetiques, Savons, August 1965.

## 2064: METHYL-3-HEXYL-2-CYCLOPENTEN-2-ONE-1

"Homodihydrojasmone".



$C_{12}H_{20}O = 180.29$

Pale straw-colored oily liquid.

Almost insoluble in water, soluble in alcohol and oils. Soluble in Propylene glycol.

This ketone, closely related to natural Jasmone, has been identified in several natural products, including Ginger.

Its synthesis falls in line with the syntheses of other relatives to Jasmone, and its odor has much in common with that ketone.

Warm-spicy, sweet-floral and diffusive, yet quite tenacious odor. Its power and floral beauty does not quite match that of *cis*-Jasmone.

It has a sweet, warm-floral-spicy, almost breadlike taste in dilutions below 5 ppm. The pleasant taste level is about 0.2 to 0.5 ppm.

Although rarely offered under its proper chemical name, this ketone finds some use in perfume compositions. Its floral power, its warmth combined with a versatile and pleasant spiciness makes it widely applicable. It blends excellently with Labdanum and Cistus-products, with Rose materials and Civet, and it gives interesting effects as part of novel topnotes, particularly with herbaceous or floral-herbaceous fragrance pictures.

Prod.:

1) from *3*-Methylcyclopenten-*2*-one-*1* plus Hexaldehyde, followed by hydrogenation.
2) from Heptyl magnesiumchloride plus Ethyl levulinate to yield the Lactone which is subsequently treated with Phosphorous Pentoxide.

4-90; 86-220;
see also: Chemical Abstracts 1955, 7554.

## 2065: METHYL-n-HEXYLETHER

*n*-Hexyl methylether.

$CH_3—O—C_6H_{13}$

$C_7H_{16}O = 116.21$

Colorless liquid. B.P. 130° C. Sp.Gr. 0.78.

Insoluble in water, soluble in alcohol and oils.

Green-ethereal, fruity odor of moderate to poor tenacity.

Apart from very occasional application in certain fresh topnotes, this ether finds mostly its place in masking odors and industrial fragrances.

Its peculiar type of green note has tempted some perfumers to use it in Jasmin and other florals, but it seems that competition from many new "green" materials is far too strong.

For masking and for room sprays, it can introduce very pleasant variations in Lavender and Hay fragrances, and its power and low cost make it attractive in certain ways.

Prod.:

1) by dehydration of Methanol plus Hexanol.
2) from Hexyl chloride plus Sodium methylate.

37-175;

## 2066: METHYL HEXYL KETONE

*n*-Hexyl methyl ketone.
*2*-Octanone.

$CH_3—CO—C_6H_{13}$

$C_8H_{16}O = 128.22$

Colorless liquid. Sp.Gr. 0.82. B.P. 173° C.

Insoluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

The comments made under the monograph "Methyl hexyl carbinol" could, to a certain extent, be made for the corresponding ketone: Enormous variations in odor description seem to indicate wide variation in olfactory (and chemical) quality of this ketone from different manufacturers. Description range from "harsh-gassy-metallic" to floral-green-fruity.

The author prefers to give a general description of a good commercial grade of the ketone, suitable for perfumery.

Pleasant, floral, but bitter-green, slightly musty-herbaceous and "unripe-Apple"-fruity odor of moderate to poor tenacity.

Bitter-camphoraceous taste in concentrations higher than 10 ppm.

This ketone, often used "in place of" Ethyl-*n*-amyl ketone for Lavender reinforcement, is by no means a substitute for the isomer ketone, although it can be used for Lavender and Lavandin with effect of increased power and diffusion. It lacks the musty sweetness and haylike herbaceousness of the *3*-Octanone.

But it has the advantage of being very inexpensive, and it is therefore used more generally in fragrances other than Lavender-Lavandin.

One peculiar combination is Methylhexylketone plus Methylacetophenone plus Benzylacetate, which may produce an extraordinarily powerful Apple-effect, sometimes useful where unpleasant odors have to be masked (cosmetic raw materials, Proteins, Sulfur, etc.).

Discrete amounts of the "good-quality" ketone are used in Reseda (Mignonette), Tuberose, Lilac, Carnation, etc.

The ketone is also used in flavor compositions for imitation Apple, and in various fruit complexes, cheese flavors, etc. Concentration is normally as low as 0.1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2802.

Prod.:

1) by oxidation of *secondary*-Octanol, obtained from Castor oil.
2) from Heptaldehyde, obtained from Castor oil.

4-90; 5-150; 7-206; 26-606; 31-80; 61-67; 66-516; 86-93; 100-519; 103-189; 103-197; 160-1130; B-I-704;

## 2067: METHYL-iso-HEXYL KETONE

*6*-Methylheptan-*2*-one.
This isomer is a component of certain commercial types of Methyl hexyl ketone.

$CH_3—CO—CH_2—CH_2—CH_2—CH(CH_3)_2$

$C_8H_{16}O = 128.22$

Colorless oily liquid. B.P. 166° C.

Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, also camphoraceous and slightly spicy-herbal odor of moderate to poor tenacity. The odor has little or no resemblance to Lavender, and is thereby distinguished from Methyl hexyl ketone. Due to its power, diffusive strength and low cost, this material has found some use in perfume compositions, mainly those intended for "heavy duty", masking, industrial uses, etc.

The odor has at times been described as "Caraway-like", but the author has searched for that note in vain when studying the material.

Prod.: by controlled hydrogenation of Methylheptenone.

86-94;

## 2068: 3-METHYL HEXYL METHACRYLATE

The title name (commercial name) is a somewhat confusing name for:
Hexyl-*3,3*-dimethylacrylate.
Hexyl-*iso*-propylidene acetate.
Hexyl-*beta*-methylcrotonate.
Hexyl-*2*-methylbuten-*2*-oate-*4*.
Hexyl senecionate.

$C_6H_{13}—OOC—CH=C(CH_3)_2$

$C_{11}H_{20}O_2 = 184.28$

Colorless mobile liquid.

Insoluble in water, soluble in alcohol and oils.

Somewhat "gassy" and very diffusive,

penetrating, warm-herbaceous and aromatic odor with a vinous note, suggestive of Chamomile and other sweet herbs. Poor tenacity.

This isomer of Hexyltiglate and Hexyl angelate finds a little use in perfume compositions, mainly in the construction of artificial essential oils, e. g. Chamomile.

It gives interesting effects as a topnote component in masculine herbaceous fragrances, and blends very well with Juniperberry oil, a material which has had a lively come-back in fragrances for Men.

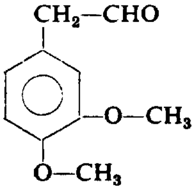
Prod.:

1) from Acetone and Malonic acid, followed by esterification.
2) by oxidation of Mesityloxide with Sodium hypochlorite, and subsequent esterification of the acid.

(Sample: Dow. Chem. Co., 1956).

## 2069: METHYL HOMOVANILLIN

*3,4*-Dimethoxy phenylacetaldehyde.
Homoveratraldehyde.



$C_{10}H_{12}O_3 = 180.21$

White crystalline material.

Very slightly soluble in water, somewhat soluble in hot water. Soluble in alcohol and oils.

Faint, sweet, warm and tenacious odor with only a remote resemblance to Vanilla. More earthy or Nut-like and balsamic.

This ether-aldehyde has been suggested for use in perfume compositions, but it has found only little more than academic interest.

Studies seem to show that the Hydroxyl-group should be in *para*-position to the Aldehyde group in material of above chemical family in order to produce a good Vanilla-like odor.

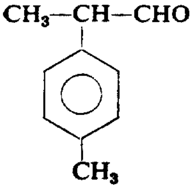
When an olfactorily important Hydroxyl-group is substituted with an Alkoxy-group, there is usually an enormous loss of odor power. In alifatic chemicals, however, there are many examples that this substitute introduces floral notes in place of sharp, powerful or pungent notes with the Hydroxyl group.

On account of sweetness, tenacity and delicate floralness, the subject chemical could find some use in perfumes of Cassie, Mimosa, Lilac and other mild floral type.

Prod.: by Methylation of Homovanillin.

## 2070: para-METHYLHYDRATROPIC ALDEHYDE

*2*-(*para*-Tolyl)-propionic aldehyde.
*para*-Methyl-*alpha*-methylphenylacetaldehyde.
*2*-(*para*-Methylphenyl)-propionic aldehyde.
*2*-(*4*-Methylphenyl)-propanal.



$C_{10}H_{12}O = 148.21$

Colorless oily liquid. Sp.Gr. 0.98.

Almost insoluble in water, soluble in alcohol and oils.

Powerful green, but also richly sweet odor of moderate tenacity. The green note is accompanied by a peculiar woody note, reminiscent of Atlas Cedarwood oil. One would be tempted to assume that such note derived from a ketonic component and not from an aldehyde.

This aldehyde is used quite widely, although never in high concentrations, in perfume compositions where green notes are agreeable to floral notes, or it may constitute part of an entirely green note in a Chypre or Lavender composition, Fougère, etc.

It gives pleasant effect and good power in Hyacinth, Lilac, Narcisse etc., occasionally in Gardenia and Honeysuckle.

Prod.: from *para*-Methylacetophenone via *para*-Methyl-phenylmethylglycidic acid.

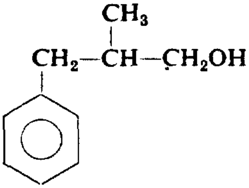
The material finds a little use in herbaceous-spicy condiment flavors, e.g. Caraway, – often in very minute amounts up to about 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.3078.

4-90; 86-93; 106-251;

## 2071: 2-METHYL HYDROCINNAMIC ALCOHOL

*2*-Methyl-*3*-phenylpropanol-*1*.
Methyl benzyl ethyl alcohol.
*beta*-Benzylpropanol-*1*.
*alpha*-Methyl hydrocinnamic alcohol.
Occasionally called "*iso*-D.M.B.C.".



$C_{10}H_{14}O = 150.22$

Colorless oily liquid. Sp.Gr. 0.98.
B.P. 241° C.

Very slightly soluble in water, soluble in alcohol and oils.

Warm, but mild, balsamic-floral odor, spicier than Hydrocinnamic alcohol, and slightly sharper. Moderate tenacity.

This alcohol, although related to well known aldehydes and esters, is comparatively rare on the perfumers' shelves. Perhaps its lack of character and its higher cost as compared to the relatives of similar odor type are factors contributing to the absence of interest in this material.

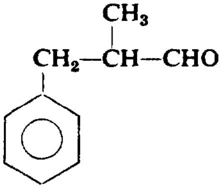
It could find use as a modifier and blender in floral and floral-Oriental fragrance types, being milder than Cinnamic alcohol and more versatile in its floral tonalities. But cost is also a factor to consider, and it cannot compete with Cinnamic alcohol in that field.

Prod.: by hydrogenation of *alpha*-Methylcinnamic aldehyde (see that monograph).

86-98; see also: 990.

## 2072: alpha-METHYL HYDROCINNAMIC ALDEHYDE

*2*-Methyl-*3*-phenyl propionaldehyde.
Do not confuse with:
*para*-Methyl hydrocinnamic aldehyde, also called:
*para*-Methyl phenylpropionic aldehyde.
(See next monograph).



$C_{10}H_{12}O = 148.21$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

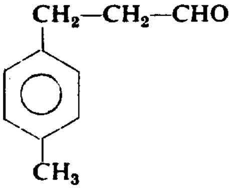
Mild and sweet, oily-floral, warm odor with a faint undertone of fruity-spicy character and a good tenacity.

This aldehyde, distinctly different from its isomer (see above) and from its unsaturated relative, Methylcinnamic aldehyde, has found a little use in perfume compositions as a modifier in balsamic-floral and spicy-floral fragrances. Its mildness makes it quite versatile, but also somewhat uninteresting as compared to the above mentioned materials which have a distinct character.

Prod.: by controlled hydrogenation of *alpha*-Methylcinnamic aldehyde which is obtained from Benzaldehyde by condensation with Propionic aldehyde under mildly alkaline, aqueous conditions.

## 2073: para-**METHYL HYDROCINNAMIC ALDEHYDE**

*4*-Methyl phenylpropionic aldehyde.
*3*-(*4*-Methylphenyl)-propionic aldehyde.



$C_{10}H_{12}O = 148.21$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, warm-floral, tenacious odor with mildly spicy undertones. Reminiscent of Heliotrope and Cassia, but overall more delicate.

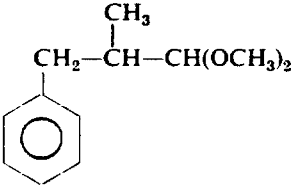
This aldehyde has been suggested for use in perfume compositions as a supporting floral or floral-balsamic or floral-spicy ingredient in Oriental fragrance types, Sweet Pea, Frangipanni, etc. or in various Fantasy fragrance types. It blends well with the Ionones, Amylsalicylate, Ylang-Ylang, Cinnamic alcohol, etc. and gives interesting depth to a Lilac, with its more delicate notes, generally preferred over Anisaldehyde or similar, harsh odorants.

Prod.: by condensation of *para*-Tolylaldehyde with Acetaldehyde, followed by hydrogenation of the unsaturated chain.

4-91; 36-1027;

## 2074: alpha-**METHYL HYDROCINNAMIC ALDEHYDE DIMETHYLACETAL**

*2*-Methyl-*3*-phenyl-*1,1*-dimethoxypropane.



$C_{12}H_{18}O_2 = 194.28$

Colorless, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet and mild, balsamic-rosy odor of great depth and warmth.

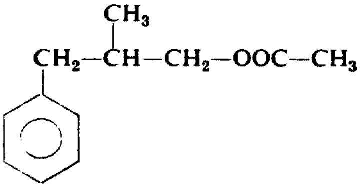
This acetal, rarely offered under its proper chemical name, finds some use in perfume compositions, particularly in floral bases as a blender/modifier. It performs very well with Phenylpropylalcohol in Rose bases, where it supports the freshness in spite of the rather heavy overall type.

It is also occasionally used in Oriental fragrance types, where it blends excellently with Patchouli, Styrax, Peru and Tolu balsams.

Prod.: from *alpha*-Methylhydrocinnamic aldehyde with Methanol by condensation in presence of a dehydrating agent.

## 2075: alpha-**METHYL HYDROCINNAMYLACETATE**

*alpha*-Methyl-*3*-phenyl propylacetate.



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm, floral-fruity, sweet odor of moderate tenacity. Resemblance to Lily, Magnolia, Lilac.

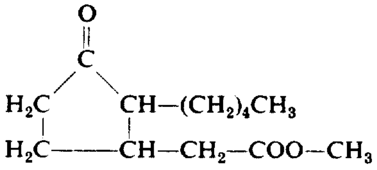
This ester, rarely offered commercially, is used in various floral fragrance types, often in connection with mildly spicy notes, e. g. in modern versions of the "Blue-Grass"-theme, or as a modifier in mildly floral fragrance types, new types of Lilac, fantasy-florals, etc.

It blends excellently with Clove bud oil, Cinnamic alcohol, the "rose alcohols", Amylcinnamic aldehyde, etc. and it gives very interesting background to "red Rose" type bases.

Prod.: from *alpha*-Methylcinnamic alcohol (see monograph) by hydrogenation followed by esterification of the alcohol in the saturated side-chain.

## 2076: METHYL HYDROJASMONATE

*2*-Amylcyclopentanoneacetic acid, Methylester.
Methyl dihydrojasmonate.
Methyl-(*2*-amyl-*3*-oxocyclopentyl)-acetate.



$C_{13}H_{22}O_3 = 226.32$

Pale straw-colored to pale yellowish or almost colorless oily liquid.
Sp.Gr. 1.00. B.P. higher than 300° C.

Very slightly soluble in water, soluble in alcohol and oils.

Warm, sweet-floral, powerful Jasmine-like and fruity odor of moderate to good tenacity.

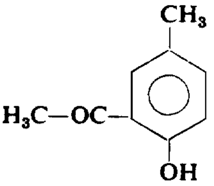
This ester, only recently brought into the market as a commercially available perfume chemical, is intended for use in artificial Jasmin absolute, Jasmin and Tuberose bases, and as a trace additive in powerfully floral fragrances. It serves as an economical substitute for Methyl jasmonate (see monograph), but does not have the overwhelming sweetness and diffusive power of that material.

Prod.: from *2*-Pentylcyclopenten-*2*-one with Ethylmalonate, followed by saponification and decarboxylation to the acid, from which the ester is obtained with Methanol.

Sample: Compagnie Parento 1968.
90-355; see also: 156-223; 163-359;
In 1969, the title ester cost nearly twice as much as Jasmin absolute from Italian concrete.

## 2077: 3-METHYL-6-HYDROXY ACETOPHENONE

*5*-Acetyl-*para*-Cresol.
"Oxymethylacetophenone" (name often used in literature).
"Isojasmone de Darzens".
*4*-Hydroxy-*5*-acetyltoluene.
*2*-Oxy-*5*-methylacetophenone.



$C_9H_{10}O_2 = 150.18$

Colorless crystals or opaque crystal mass.
M.P. 49° C.
Insoluble in water, soluble in alcohol and oils.

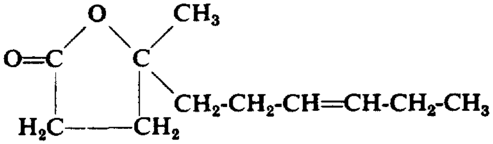
Sweet-herbaceous, floral-woody odor of considerable tenacity. The floral notes are only detectable when the material is incorporated in a composition, while the sweet-woody-herbaceous notes are predominant in the material itself.

This ketone-phenol has been suggested for use in powerful floral compositions. Although one trade name implies a Jasmin-type effect, the author finds that the material is useful in Mimosa, Cassie, Lilac and many other florals, not only Jasmin. It blends well with Labdanum and Cedrus Atlantica (Moroccan Cedarwood oil) in the novel type of "Oriental" fragrance, and it supplies solid undertones in Lavender or other herbaceous types.

163-210; 163-368;
see also: Chemisches Centralblatt 1956, page 1545, and "la Parfumerie Moderne" 1951, vol. 22, page 27.

## 2078: 4-METHYL-4-HYDROXY-7-DECENOIC ACID, LACTONE

Hexenyl-*gamma*-valerolactone (misleading name).
"Undecenolide-*1,5*"
Methyldecenolide-*1,4*.
(The *cis*- and *trans*-forms of an isomer, *alpha*-Hexenyl-*gamma*-methylbutyrolactone, are known, but apparently not interesting to the perfume industry).



$C_{11}H_{18}O_2 = 182.27$

Colorless or pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful oily-fruity, heavy Peach-like odor of outstanding tenacity. Not as fatty-grassy as Undecanolide-*1,4*, and not quite as tenacious, but in dilution more natural Peach-like.

This Lactone is rarely offered commercially, but finds some use as part of various specialties and bases sold under trade names (usually indicating the "fruity" note in the name).

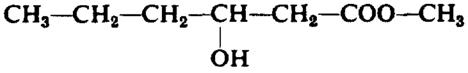
Its high cost of production is a serious drawback for this otherwise interesting chemical. Unless new methods of synthesizing the material at considerably lower cost are developed, it is most conceivable that this chemical will not become widely used.

Prod.: from *cis-3*-Hexenyl chloride plus *cis-3*-Hexenyl iodide with Acetopropionic ester.

31-176; 31-177; 86-59;

## 2079: METHYL-3-HYDROXYHEXANOATE

Methyl-*3*-hydroxycaproate.
*beta*-Hydroxyhexanoic acid, Methylester.



$$CH_3{-}CH_2{-}CH_2{-}\underset{\displaystyle OH}{\underset{|}{CH}}{-}CH_2{-}COO{-}CH_3$$

$C_7H_{14}O_3 = 146.19$

Colorless liquid.

Oily-ethereal, powerful, fruity-winey odor of considerable radiation. Moderate to poor tenacity.

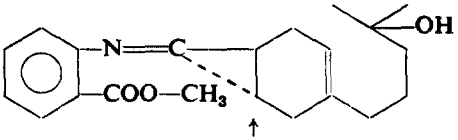
This hydroxyester has been developed mainly for the purpose of "reconstituting" the flavor in processed Orange juice. The ester forms part of a complex, often added to the Orange juice in order to compensate for the loss of certain flavor components during the processing.

Prod.: The acid is prepared from Methyl-*n*-propylketone plus *alpha*-Bromoacetic ester (or *alpha*-Chloroacetic ester) in presence of Zinc (or Magnesium).

Journal of Food Science 29, 790 (1964).

## 2080: METHYL-N-(4-(4-HYDROXY-4-METHYLPENTYL)-3-CYCLOHEXENYL-METHYLIDENE))-ANTHRANILATE

"Lyral-Methylanthranilate" (Schiff's base).



including the isomer

$C_{21}H_{29}NO_3 = 343.47$

Intensely yellow, viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Very sweet and extremely tenacious floral odor of Magnolia-Orangeblossom-Acacia type.

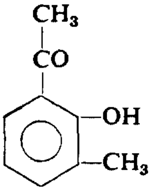
This condensation product, developed as a routine from the successful floral aldehyde, Lyral, has not shown any unusual characteristics and does not seem to offer distinctly new notes to the perfumer.

Prod.: by condensation of Lyral and Methylanthranilate.

Lyral, see: Methyl hydroxyamyl cyclohexene carboxaldehyde (No. 1754).

## 2081: meta-METHYL-ortho-HYDROXYMETHYL PHENYLKETONE

*2*-Hydroxy-*3*-methylacetophenone.
*3*-Methyl-*2*-hydroxyacetophenone.



$C_9H_{10}O_2 = 150.18$

White crystals.

Insoluble in water, soluble in alcohol and oils.

Warm floral-herbaceous odor, suggestive of certain notes of Jasmin.

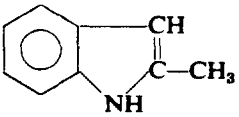
This ketone, rarely offered under its proper chemical name, is used in perfume compositions for its warm-floral effect and herbaceous character, useful in Jasmin, Tuberose, Chypres, Oriental fragrance types, etc. It is tenacious and stable in soap, and it blends excellently with all Labdanum products for Chypres, with Amylcinnamic aldehyde for Jasmin undertones, and with the Coumarins for herbaceous fragrances.

Prod.: by Darzen's type synthesis from *ortho*-Cresylacetate by heating with Aluminum chloride.

4-241;

## 2082: alpha-METHYL INDOLE

*iso*-Skatole.
*2*-Methylindole.



$C_9H_9N = 131.18$

White crystals. M.P. 62° C. B.P. 273° C.

Almost insoluble in water, soluble in alcohol. The solutions in oils may show violet-bluish-green fluorescence.

Powerful and diffusive, yet very tenacious animal-indolic odor, fresher and not as repulsive as Skatole. In fact, the animal notes of this isomer are rather attractive, not at all fecal.

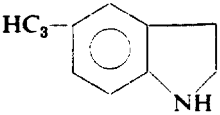
This interesting chemical, widely used under trade names, finds a place in many compositions where a special variation of the Indole type odor is desirable. It is also claimed that this derivative shows less tendency of discoloration than any other commercially available related product.

Its power is about equal to that of Indole, but it seems to lack the pungency, often connected with traces of naphthalenic type of off-odor in commercial grades of Indole. Which is only to the advantage of this derivative.

Prod.:
1) from Acetone phenylhydrazone by heating with Zinc chloride.
2) from *N*-Acetyl-*ortho*-toluidine by heating with Sodamide to about 250° C. – or by heating with Sodium and Copper in boiling Diethyl aniline.

4-91; 69-76; 69-84; 69-86; 95-204; 95-224;
See also monograph. Skatole (= *beta*-Methyl indole).

## 2083: 5-METHYLINDOLE



$C_9H_9N = 131.18$

White crystals. M.P. 59° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

The odor of this material is similar to that of Indole, but not as powerful and not nearly as floral in use-dilution. It is also weaker than Skatole and does not have the Civet character of that isomer. It resembles more the 2-Methyl indole except for the lack of floral power.

Although this isomer has some advantage in lesser tendency of discoloring with many perfume materials otherwise incompatible with pure Indole, it has failed to attract the attention of the creative perfumer who has become adjusted to the drawbacks and hazards in use of Indole.

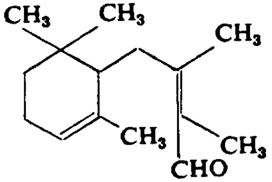
This isomer is rarely offered under its proper chemical name.

Prod.: by the Fischer type synthesis, starting from *para*-Toluidine.

69-84;

## 2084: alpha-METHYL IONAL

Commercially often called:
Methyl ionyl acetaldehyde:
*4*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-*2,3*-dimethyl-*2*-buten-*1*-al.
The commercial product is not a well-defined, single chemical.



$C_{15}H_{24}O = 220.36$

Yellowish or straw-colored viscous oil.
B.P. 270° C.

Practically insoluble in water, soluble in alcohol and oils.

Intensely sweet, "jam-like" fruity preserve-type odor with some resemblance to the odor of dried figs. Excellent tenacity with woody undertones.

Sweet-fruity, fig-like and mildly woody taste in concentrations below 10 ppm.

This peculiar material, often marketed under trade names, has found some use in perfumery for its great tenacity, sweetness and ability to blend fruity with woody notes.

Its odor bears considerable similarity to the odor of the Ionone glycidates (see Ionone methyl glycidate), but is generally fresher, more sweet-woody. Variations in odor of products from different manufacturers add to the confusion and the general impression of the true odor type. Such variations and anomalies may result in a conscious or subconscious "boycott" from the part of the perfumer, who prefers to use materials obtainable from several sources.

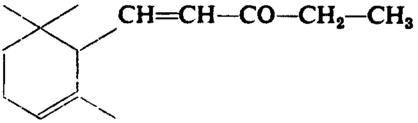
The title material has never become a very important perfume material, but its peculiar similarity to fig-flavor could make it an interesting flavor item if the subject material could be approved as G.R.A.S. or generally approved by the authorities for food flavor use.

Prod.: from Acetaldehyde and *alpha*-Methyl ionol.

86-95; 163-50; 163-222; 163-361;

## **2085:** alpha-n-**METHYL IONONE**

*alpha*-Methylionone.
*5*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*4*-penten-*3*-one.
*alpha*-Cyclocitrylidene butanone.
"Cetone Alpha",
- and many other trade names.



$C_{14}H_{22}O = 206.33$

Almost colorless or pale straw-colored oily liquid. Sp.Gr. 0.93. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Commercial Methylionones, unless specifically marketed as "*gamma*-Methylionone", usually contain the *alpha-n*-isomer as the chief component.

Floral and sweet-oily odor of moderate tenacity.

This Methylionone is used quite extensively in perfume compositions as a blender/modifier and background note in floral or floral-Oriental compositions, Mimosa-Cassie bases, in numerous versions of "Quelques-fleurs" type fragrances or "l'Origan"-types, Chypres, etc.

For further comments on the odor of Ionones and Methylionones, read E. S. Maurer (103-268/269) explaining part of the reasons for the difficulty in discriminating between them or describing their odor nuances.

The manufacturers of Ionones and Methylionones must have realized this difficulty, since the trend has been towards a simplification by strictly reducing the number of types of Methylionone marketed by the individual manufacturer.

The subject material is also used in flavor compositions as part of imitation Raspberry and other berries, Violet and various floral types and in some fruit complexes and "Sen-Sen" type licorice flavorings.

The concentration is usually low, about 0.2 to 8 ppm in the finished product.

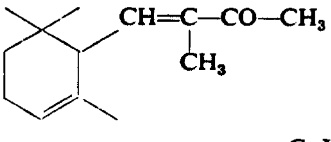
Prod.: by condensation of Methylethyl ketone with Citral, and cyclization of the resulting Pseudomethylionone. Cyclization may be carried out with Boron trifluoride or other agent.

G.R.A.S. F.E.M.A. No.2711.

5-176; 96-168; 103-268; 106-254; 156-198;

## **2086:** alpha-iso-**METHYL IONONE**

*iso*-Methyl-*alpha*-ionone.
"*gamma*"-Methylionone. (See also mono: graph: *gamma*-Methylionone).
Iraldeine Gamma.
Noviraldiol.
Raldeine Gamma.
- and many other trade names.
*4*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*3*-methyl-*3*-buten-*2*-one.



$C_{14}H_{22}O = 206.33$

Almost colorless or pale straw-colored oily liquid. B.P. 230° C. Sp.Gr. 0.93.

Insoluble in water, soluble in alcohol and oils.

The odor of this isomer is generally considered more attractive than any other Methylionone, perhaps with the exception of the *beta-iso*-Methylionone, so-called *delta*-Methylionone. It is extremely versatile in character, and effects ranging from sweet floral to tobacco-like or woody are obtainable with various grades of subject material. The most refined grades, which are quite expensive, often show a very attractive "creamy" topnote and a most uniform, powdery-sweet dryout performance. This type of Methylionone can support floral notes in Ylang-Ylang as well as woody notes in Vetiver, or leathery notes in Salicylates, etc. Certain types of perfume contain up to 25% or more of this material. Many soap perfumes are based upon a large volume of common-grade Methylonone with the subject isomer as predominant component.

For olfactory description of Ionones and Methylionones, see also E. S. Maurer: 103-268/269.

The subject material finds some use in flavor compositions, not only in many berry types and Violet and other florals, but in Pineapple, Muscatel, Nut, Pistacio, fruit complexes, etc.

Concentrations vary from 0.05 to 10 ppm in the finished product.

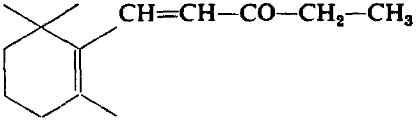
G.R.A.S. F.E.M.A. No.2714.

Prod. by condensation of Citral with Methyl ethyl ketone, followed by cyclization of the Pseudomethylionone. Variations in the second step largely control the ratio of isomers in the Methylionone.

5-176; 103-268; 106-252; 156-198;

## 2087: beta-n-**METHYL IONONE**

*beta*-Methylionone.
*5*-(*2,6,6*-Trimethyl-*1*-cyclohexen-*1*-yl)-*4*-penten-*3*-one.
Cetone Beta.
Iraldeine Beta.
Raldeine Beta -
and numerous other trade names.



$C_{14}H_{22}O = 206.33$

Almost colorless or pale straw-colored oily liquid. B.P. 242° C.

Insoluble in water, soluble in alcohol and oils.

Woody-warm odor, generally considered to be a *beta*-Ionone type. For description of the odor of Methylionones, see also: E. S. Maurer: 103-268/269.

This isomer is the least important of the commonly available Methylionones. Its odor type does not tempt the perfumer to use it very extensively, particularly since *beta*-Ionone is commercially available at a very attractive price, being an intermediate in the manufacture of synthetic Vitamin A.

It finds a little use in flavor compositions, partly as a modifier for *beta*-Ionone in Raspberry imitations, also in Strawberry and other berries, Orange and other Citrus imitations, Violet and other floral types and in certain fruit complexes.

Concentration is normally about 2 to 10 ppm in the finished product.

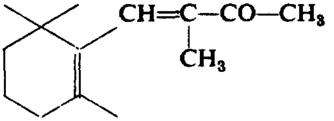
G.R.A.S. F.E.M.A. No.2712.

Prod.: by condensation of Citral with Methyl ethyl ketone, followed by cyclization. Solvents and acids used in the cyclization process will largely influence the proportion of *beta*-isomer in the yield.

5-176; 103-268; 106-252; 156-198;

## **2088:** beta-iso-**METHYL IONONE**

*iso*-Methyl-*beta*-ionone.
*4*-(*2,6,6*-Trimethyl-*3*-cyclohexen-*1*-yl)-*3*-methyl-*3*-buten-*2*-one.
"*delta*"-Methylionone.
Rhodione Methyl Delta.
Ironal Methyl Delta.
Raldeine Delta.
Iraldeine Delta,
– and many other trade names.



$C_{14}H_{22}O = 206.33$

Almost colorless or slightly yellowish oily liquid. B.P. 232° C.

Insoluble in water, soluble in alcohol and oils.

Light and warm-woody, floral and at the same time Ambregris-like odor of moderate tenacity. Odor varies in products from different suppliers. An absolutely pure isomer without other isomers present is not commercially available.

This is a rather expensive, but highly desirable isomer of the Methylionones. Its mildly animal (Ambregris-like) notes have made the material particularly interesting as a base for luxury perfumes, many of which contain a high percentage of subject material.

See also remarks about Methylionone odors under literature 103-268. (See also: Cyclocitrylidene methylpentanone).

The material finds limited use in flavor compositions, mainly in berry or fruit flavors, and in floral types. Concentration is about 0.5 to 3 ppm in the finished product.

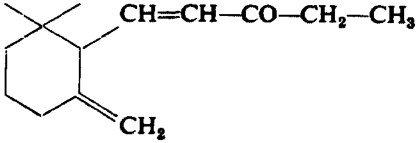
G.R.A.S. F.E.M.A. No.2713.

Prod.: see previous monographs. The *beta-iso*-Methylionone forms a small part of the mixture normally obtained in the final process. It is possible to make changes in conditions thus favouring the formation of subject isomer, but it never appears as the chief component of the reaction mixture.

5-176; 103-268; 106-252; 156-198;

## **2089:** gamma-n-**METHYL IONONE**

*gamma*-Cyclocitrylidene butanone.
*5*-(*2*-Methylene-*6,6*-dimethylcyclohexyl)-*4*-penten-*3*-one.
Do not confuse with "*gamma*" Methylionone (*iso*-Methyl-*alpha*-ionone).



$C_{14}H_{22}O = 206.33$

Almost colorless or pale straw-colored oily liquid. B.P. 252° C. Sp.Gr. 0.93.

This isomer, although regularly occurring in commercial grade "Methyl ionone" is rarely offered as such. It is not a trace component, but may amount to 10% or even more of the Methylionone mixture.

An odor description of this (and the *iso*-) is therefore of little value unless based upon a commercially available sample of high-purity single isomer.

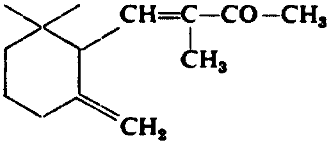
The description of subject isomer is included merely for the completion of the monographs on Methylionones.

Future research may reveal that these isomers are of substantial perfumery value, but it is still too early to predict this.

156-198; 156-203; 156-208;

## 2090: gamma-iso-METHYL IONONE

*gamma*-Cyclocitrylidene butanone.
*4*-(*2*-Methylene-*6,6*-dimethylcyclohexyl)-*3*-methyl-*3*-buten-*2*-one.
Not identical to "*gamma*"-Methylionone (see monograph: *alpha-iso*-Methylionone).



$C_{14}H_{22}O = 206.33$

Pale straw-colored or almost colorless oily liquid. B.P. 255° C.

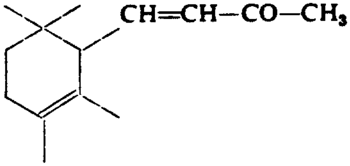
This isomer, usually one of the "larger by-ingredients" in commercial Methylionone, is rarely offered separately in a pure state. Its presence in commercial grade Methylionone is of no great disadvantage since it does not reduce the "total ketone" value of the product, and its odor has some similarity to that of the presently desirable isomer, *alpha-iso*-Methylionone.

See also notes under previous monograph.

156-198; 156-203; 156-208; 156-210;

## 2091: 4-METHYL IONONE

*4*-(*2,3,6,6*-Tetramethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.
"Velvione" (Rhodia).



(*alpha*-structure, most common isomer).

$C_{14}H_{22}O = 206.33$

Pale straw-colored or almost colorless oily liquid. B.P. 270° C. Sp.Gr. 0.93.

Insoluble in water, soluble in alcohol and oils.

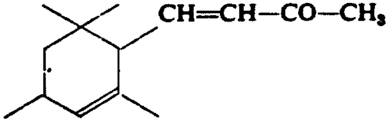
The odor of this isomer of *alpha*-Irone seems to be stronger than that of *alpha*-Ionone, but weaker than that of *alpha*-Irone. The type is similar to that of *alpha*-Ionone.

Since the cost of production of this material is so much higher than that of *alpha*-Ionone, it is not likely that it will become a very popular item. It is included in this work mainly for reasons of completing the section on isomers of Methylionone.

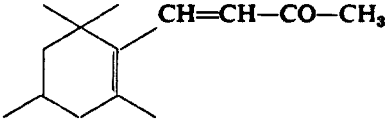
5-341; 86-95; 159-448;

## 2092: 5-METHYL IONONE

The commercial product is normally a mixture of almost equal parts of
*5*-Methyl-*alpha*-ionone and *5*-Methyl-*beta*-ionone.



*alpha*-isomer
*4*-(*2,4,6,6*-Tetramethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.



*beta*-isomer
*4*-(*2,4,6,6*-Tetramethyl-*1*-cyclohexen-*1*-yl)-*3*-buten-*2*-one.

$C_{14}H_{22}O = 206.33$

Almost colorless or pale straw-colored oily liquid. B.P. 277° C. Sp.Gr. 0.91.

Insoluble in water, soluble in alcohol and oils.

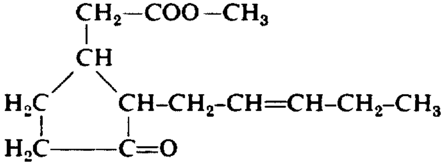
Ionone-like odor, but more floral than *alpha*-Ionone. However, it is weaker than *4*-Methyl ionone and *6*-Methylionone (Irone).

Apparently of little interest to the perfumer, this material is mentioned for academic interest and for the completion of the Methylionone series.

86-95; 159-448;
(see also: *alpha*-Irone.)

## 2093: METHYL JASMONATE

*2*-Pentenylcyclopentanone-*3*-acetic acid, Methylester.
*2*-(*cis*-Penten-*2'*-yl)-*3*-oxo-cyclopentane acetic acid, Methylester.



$C_{13}H_{20}O_3 = 224.30$

Colorless oily liquid. B.P. higher than 300° C. Sp.Gr. 1.02.

Almost insoluble in water, soluble in alcohol and oils.

Powerful floral-herbaceous, sweet-tenacious odor representing typical background notes of Jasmin absolute. This ester has been identified in Jasmin absolute (Helvetica Chim. Act. 45, 1962, page 686).

Although this material is an almost obvious candidate for work on improved artificial Jasmin absolute, its cost is still too high to allow extensive and free use. Most perfumers realize that a good artificial Jasmin absolute must run a production cost of considerably more than $ 8 or 10 per kilo, but they also face the fact that the very expensive artificial Jasmins would be limited to "interior" use in bases, perfumes, etc. and not for sale as such.

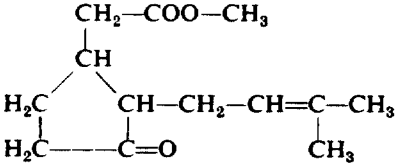
It is once more the "vicious circle" against the introduction of a new perfume material: if it could only come into volume demand, it could be sold at a very reasonable price. If it remains very expensive, it will never come into volume use. Usually, the manufacturer must yield to this hard fact and reduce the cost before his initial expenses are paid, hoping that increased volume sales will compensate for the early price reduction.

Prod.: from Muconic acid via *3*-Oxo-cyclopentane acetic acid.

90-353; 90-667; 105-588; 156-226; 163-361;

## 2094: METHYL-iso-JASMONATE

*2*-*iso*-Pentenyl cyclopentanone-*3*-acetic acid, Methylester.



$C_{13}H_{20}O_3 = 224.30$

Colorless oily liquid. Sp.Gr. 1.01.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral, tenacious, Jasmin-like odor.

This ester, commercially available at a cost much below that of Methyl jasmonate, has been suggested as a substitute for the naturally occurring ester. However, it does not have quite the same power in its sweetness, and its floral notes are somewhat harder than those of the Methyljasmonate. These slight drawbacks must be weighed against the considerable cost difference.

As long as Methyljasmonate remains at its very elevated cost, there is a good chance that the isomer will find use in various types of artificial Jasmin absolute, Tuberose, Gardenia and many other heavy-sweet floral types.

(Sample: Compagnie Parento, 1967).

## 2095: METHYL LAURATE

Methyl dodecylate.
Methyl dodecanoate.

$CH_3(CH_2)_{10}COO—CH_3$

$C_{13}H_{26}O_2 = 214.35$

Colorless, slightly oily liquid. Sp.Gr. 0.87. B.P. 262° C.

Solidifies in the cold, melts at 5° C.

Insoluble in water, soluble in alcohol and oils.

Oily-fatty, winey and slightly floral odor with remote resemblance to Violet. Relatively diffusive and powerful, yet quite tenacious.

This ester finds some use in perfume compositions, partly as a component of Orris and Violet notes, partly in Mimosa, Cassie, Lilac, Tuberose, Rose, Jasmin and other florals in which a fatty, "petal-like" note may be desirable.

The ester finds a little use in floral flavor types at very low concentration, normally about 0.02 to 1 ppm in the finished product.

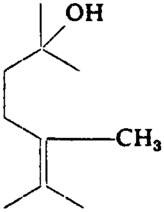
G.R.A.S. F.E.M.A. No.2715.

Prod.: by direct esterification of Methanol with Dodecanoic acid, preferably under azeotropic conditions.

7-276; 4-93; 86-96; 90-214; 103-81;

## 2096: METHYL LINALOOL

"*3*-Methyl linalool".
*3,6,7*-Trimethyl-*1,6*-octadien-*3*-ol.
"Cayenol" (Rhodia).
This material is often confused with:
Methyl linalyl ether (sometimes called "Methyl linalool") – see monograph.
Ethyl linalool (an isomer of the title material) – see monograph.



$C_{11}H_{20}O = 168.28$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Floral-woody odor, slightly sweeter, less woody and more floral than Linalool, but also much weaker. Fair tenacity.

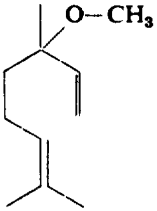
This alcohol is included in the present work mainly for the sake of completing the description under the name "Methyl linalool".

The title material is too expensive to be of interest to the perfumer, particularly since the recent development of very low-cost Linalool and many interesting derivatives thereof.

4-93; 86-96; 163-51; 163-223;

## 2097: METHYL LINALYL ETHER

Linalool methylether.
Linalylmethylether.
"Methyllinalool".
*3*-Methoxy-*3,7*-dimethyl-*1,6*-octadiene.
*3*-Methyl linalool.
Do not confuse with Ethyl linalool, which is actually Methyl linalool, or Homo-linalool (see monograph: Ethyl linalool).



$C_{11}H_{20}O = 168.28$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Light, floral-herbaceous, slightly green-woody odor with a mildly camphoraceous undertone. Without being sharp or pungent, it has some resemblance to the odor of Linalool oxide.

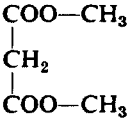
This ether, occasionally available, but rarely in a pure state, has been suggested for use in perfume compositions. It could be used in floral as well as in herbaceous types, since it blends equally well with Bergamot, Lavender, Clary Sage and with Amylsalicylate, Citronellol, Geraniol, Linalyl esters, etc.

Its tenacity is rather poor, and it demands solid fixation in compositions.

Prod.: by isomerization of Geraniol in methylalcoholic environment. (Several other methods are known and used).

## 2098: METHYL MALONATE

Dimethyl malonate.
Dimethyl propane dioate.



$$\begin{array}{l} COO-CH_3 \\ | \\ CH_2 \\ | \\ COO-CH_3 \end{array}$$

$C_5H_8O_4 = 132.12$

Colorless liquid. Sp.Gr. 1.15. B.P. 181° C.

Very slightly soluble in water, soluble in Propylene glycol, alcohol and oils.

Ethereal-fruity, relatively diffusive odor of moderate to poor tenacity.

This ester finds limited use in flavor compositions, where it may substitute or modify the Ethylester, somewhat more common in use.

The subject ester adds fresh-ethereal green notes to Apple, Gooseberry, Rhubarb, Apricot, Banana, etc.

Prod.: by direct esterification of Methanol with Malonic acid using azeotropic conditions.

7-276; 26-518; 31-126; 100-679; 160-1084; B-II-572;

## 2099: METHYL MERCAPTAN

Methanethiol.

$CH_3SH$

$CH_4S = 48.11$

A colorless gas. B.P. 6° C. Liquid under pressure or at low temperature. Methyl mercaptan hydrate is a white crystalline material. Sp.Gr. 0.87 (liquid).

The gas is slightly soluble in water, however, it decomposes slowly in aqueous solution. Soluble in alcohol and oils.

Odor of rotten cabbage, very diffusive and objectionable.

This material is formed by decomposition (fermentation, etc.) of various natural proteins.

It finds some use in flavor compositions, but more in the "reconstitution" of Coffee flavor. Particularly in products made from botanical material other than Coffee beans, e. g. Corn or Chicory.

The concentration used is normally about 0.1 to 1 ppm, but in treatment of Corn-coffee it may be as high as 5 to 8 ppm.

In spite of the extremely repulsive odor of this material, the human tolerance towards Methyl mercaptan is very high. Isolated cases of sickness from inhaling the gas are generally ascribed to psychological objection to the odor. The material is NOT classified as toxic.

G.R.A.S. F.E.M.A. No.2716.

Prod.:
1) from Sodium methylsulfate plus Potassium sulfhydrate.
2) from Methanol plus Hydrogen sulfide with catalyst.

66-347; 100-664; 159-28; 160-1098;

## 2100: 4-METHYL MERCAPTOBUTYLAMINE

$CH_3—S—CH_2—CH_2—CH_2—CH_2NH_2$

$C_5H_{13}NS = 119.23$

Colorless or pale yellowish liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Intensely "fishy", penetrating odor reminiscent of cooked lobster or crayfish. In high concentration repulsive and decay-like, but at concentrations (liquid form) below 0.01 %, the odor can be more justly evaluated.

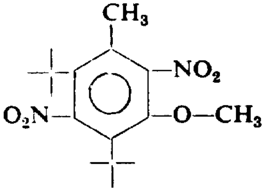
This material has been mentioned in literature because of its odor similarity to lobster and crayfish, but the author is not aware of any commercial use of the amine.

It is included in this work partly as an example of a rare type of odorant, partly because the corresponding aldehyde:
*4*-Methyl mercaptobutyraldehyde (Methyl thiobutanal)
is known and used for its meat-and soup-like flavor in extreme dilution.

The lowest member of the alkylamines, Methylamine, is also known for its odor of boiled lobsters.

(See: Der Parfumeur, 1939, page 653).
(See also: 159-424).

## 2101: 1-METHYL-3-METHOXY-4,6-DI-tertiary-BUTYL-2,5-DINITROBENZENE



$C_{16}H_{24}N_2O_5 = 324.38$

Yellowish crystals.

Insoluble in water, poorly soluble in cold alcohol, soluble in most perfume oils at the rate of 5 to 15 %.

Sweet, woody-musky odor with mildly camphoraceous undertones. The odor appears weaker than that of Musk Ambrette, less sweet, yet not Ambre-like. The tenacity is almost equal to that of Musk Ambrette.

This Nitromusk was developed from "Ambral" (Givaudan) – see monograph of *2,4*-Di-*tertiary*-butyl-*5*-methoxybenzaldehyde, which was the first Benzene-derived, Nitrogen-free chemical to display a pleasant musk-like odor. The Mono-nitro-derivative was odorless, but the title material was considered interesting at the time of discovery.

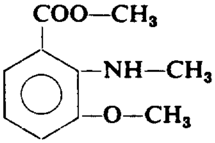
The development of Nitrogen-free musks then took such speed and produced such interesting materials, that the title material along with many similar Nitromusks practically vanished from the perfumer's shelf again. Only five Nitromusks can be classified as important in volume and frequency of use today, and the title material is not one of them.

(See also the "Givaudanian", March 1968, Mr. T.F. Wood, pages 3-5).

Prod.: from a by-product obtained in the manufacture of Musk Ambrette. Musk Ambrette has one *tertiary*-Butyl group less than the subject material.

## 2102: METHYL-3-METHOXY-2-METHYL-AMINOBENZOATE

"Damascenine".
"*3*-Methoxy dimethylanthranilate".
Methyl-*2*-methylamino-*3*-methoxybenzoate.



$C_{10}H_{13}NO_3 = 195.22$

Almost colorless or pale straw-colored liquid. Solidifies in the cold to an opaque crystalline mass or white crystals. M.P. 26° C. B.P. 271° C.

Practically insoluble in water, soluble in alcohol and oils. The diluted solutions show a beautiful blue fluorescence.

Fruity-winey, Grape-like and Brandy-like odor, rather heavy-sweet and slightly animal, with good tenacity. The overall picture bears some resemblance to Cognac oil and Ambrette-seed absolute with a fruit-jam-like undertone.

Sweet, heavy-fruity Grape-like and Wild Strawberry-like taste with a pungent floral undertone.

This chemical, absent from most perfume and flavor laboratories, belongs to a large group of perfume and flavor raw materials enjoying much more fame through the talk and stories about them, than from the actual use of them. It is probably true and justified when many perfumers and flavorists claim that they do not need this material, but for the few people who are familiar with it, and those experimenting out of endless curiosity, it is an intriguing raw material.

It could find use in exotic floral compositions and in variations of Citrus colognes, in novel topnote complexes with green-winey odorants, etc.

The material could find many uses in flavor compositions, not only in variations of Strawberry, but also Grape and "Tutti-frutti", wine, Cognac, etc.

Out of the few samples studied over many years, the author definitely prefers those prepared from the Nigella Damascena oil. Considerable care must be taken in purifying the intermediates in the preparation of synthetic Damascenine.

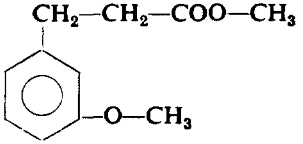
Prod.:

1) from *ortho*-Hydroxybenzoic acid by Methylation followed by Nitration, Reduction, Aminomethylation and Esterification.
2) from *8*-Hydroxyquinoline by Methylation, Oxidation, De-formylation and Esterification.
3) by isolation from the essential oil of Nigella Damascena which contains about 8 to 11 % of subject material.

5-304; 90-806; 95-190; 105-788; 140-156; 104-439;

## 2103: METHYL-(meta-METOXYPHENYL)-PROPIONATE

*3-(meta*-Methoxyphenyl)-methylpropionate.
Methyl-*meta*-methoxyhydrocinnamate.



$C_{11}H_{14}O_3 = 194.23$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

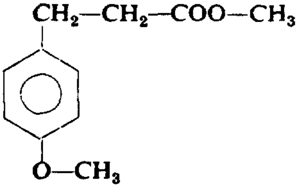
Sweet-balsamic and mildly fruity odor of good tenacity.

This ester is rarely seen in price lists, and not often found in a perfume laboratory. But it has been suggested, and is occasionally used, in perfume compositions, particularly those of Oriental type, or fruity-floral types.

The *para*-isomer is somewhat better known in perfumery (see next).

## 2104: METHYL-(para-METHOXYPHENYL)-PROPIONATE

Methyl anisyl propionate.
Methyl-*para*-methoxyhydrocinnamate.
*3-(para*-Methoxyphenyl)-methylpropionate.



$C_{11}H_{14}O_3 = 194.23$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very sweet, balsamic-spicy, warm and tenacious odor. The main difference from the *meta*-isomer is the lack of fruity notes, and the increase in sweetness and warmth.

This ester, although rare, finds some use in perfume compositions as a modifier/blender in Oriental fragrance types, heavy florals, Mimosa, Gardenia, etc.

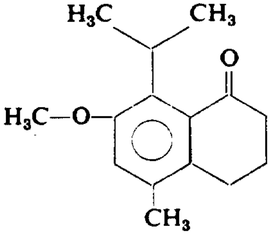
The Ethylester of the unsaturated acid occurs in Nature, and so does the acid itself, but the title material is usually prepared the synthetic way.

Prod.: from Anisaldehyde by condensation with Methylacetate in presence of Sodium. The resulting Methylether of *para*-Cumaric acid methylester is subsequently hydrogenated to the title material.

See also: 1287;

## 2105: 5-**METHYL**-7-**METHOXY**-8-iso-**PROPYL**-alpha-**TETRALONE**

*1*-Methyl-*3*-methoxy-*4*-*iso*-propyl-*8*-tetralone-*II*.



$C_{15}H_{20}O = 216.33$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Very tenacious, dry-sweet, woody odor, with a minty-camphoraceous note which makes it somewhat harsh. The suggested "Sandalwood" character is more perceptible and easier to appreciate in dilution or in composition.

The title material was developed many years ago and at that time suggested for use as a Sandalwood material. It has apparently lost most of its importance, particularly in view of the many and better materials later developed and widely marketed.

Prod.: via Friedel-Craft's synthesis using the acid chloride, followed by cyclization.

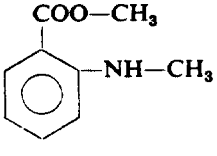
159-415;

See also monographs:

*1,1,2*-Trimethyltetralone-*3*.
*7*-*tertiary*-Butyl-*alpha*-tetralone.
*8*-*tertiary*-Butyl-*5*-methyl-*alpha*-tetralone.
*8*-*tertiary*-Butyl-*alpha*-benzosuberone.
*iso*-Bornyl methoxycyclohexanol.
*3*-Methyl-*4*(*4'*-*iso*-propylcyclohexyl)-butan-*2*-one.

## 2106: METHYL-N-METHYLANTHRANILATE

*2*-Methylamino methylbenzoate.
"Dimethyl anthranilate".



$C_9H_{11}NO_2 = 165.20$

Colorless liquid, solidifying in the cold, melting at 19° C. B.P. 256° C. Sp.Gr. 1.12 (liquid).

Practically insoluble in water, soluble in alcohol and oils.

Musty-floral, sweet and rather heavy Orangeblossom-Mandarin-peel like odor, winey-fruity undertones. Fair to good tenacity. Overall less harsh than Methylanthranilate. It should be added to the last remark, that certain brands of Methylanthranilate appear on the market in exceptionally high grade of purity, in free flowing white crystals and with a floral odor definitely superior to that of the common grade Methylanthranilate. Such grades compare favourably with the "Dimethylanthranilate" as far as "musty" notes are concerned.

On the other hand, there are still certain grades of subject material ("Dimethylanthranilate") on the market containing substantial amounts of "Mono"methylanthranilate. Such variations in quality obviously influence the evaluations of one ester versus the other.

The taste of this ester is somewhat milder and softer than that of Methylanthranilate, not quite as typical of "Concord"-grapes, more "berry"-like. It is also possible to use this ester at much higher concentration without the risk of producing an overly "chemical" taste.

The ester finds extensive use in perfumery, particularly in soap and detergent, shampoo and various cosmetic perfumes. It shows little or no tendency of discoloration, and it will not form "Schiff's bases" with the aldehydes, etc. such as observed with Methylanthranilate. It is therefore often used to replace the Mono-ester in soap perfumes where it can lend a similar effect at a slightly higher cost.

It is also used widely in flavor compositions, not only in Grape imitation, but generally in "Tutti-frutti" flavor, Citrus blends (Tangerine, Mandarin, etc.). The concentration is normally about 4 to 20 ppm in the finished product, but it may be as high as 7000 ppm in chewing gum (which means that it constitutes the major part of the flavor oil in the gum).

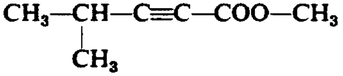
G.R.A.S. F.E.M.A. No.2718.

Prod.: from *N*-Methyl isatoic anhydride and Methanol.

5-292; 26-608; 34-1012; 68-581; 90-803; 103-164; 106-135; 140-156; 156-41; 160-810; B-XIV-324;

## 2107: METHYL-3-METHYL-n-BUT-1-YNE CARBONATE

An isomer of Methyl pentin carbonate (Methyl hexynoate).



$$CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-C\equiv C-COO-CH_3$$

$C_7H_{10}O_2 = 126.16$

Colorless liquid. B.P. 164° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and "gassy-green", diffusive odor, in extreme dilution leafy-green, but still sharp, almost pungent.

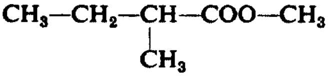
The subject ester was developed among many isomers and homologues in search of more interesting members of the acetylenic ester family. This particular ester, however, seems to have failed in the competition with higher homologues, and particularly with the modern Hexenyl esters.

Prod.: from *iso*-Valeric aldehyde via *3*-Methyl-*n*-but-*1*-yne to the acid, followed by esterification.

5-245;

## 2108: METHYL-2-METHYLBUTYRATE

Methyl methylethylacetate.
Methyl-*2*-methylbutanoate.
Methyl-*active*-valerate.



$$CH_3-CH_2-\underset{\displaystyle CH_3}{\underset{|}{CH}}-COO-CH_3$$

$C_6H_{12}O_2 = 116.16$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Pungent ethereal-fruity odor of poor tenacity.

Sweet-fruity taste with a "fermented" and Apple-like note in dilutions below 20 ppm.

This ester, only recently appearing on the market, finds limited use in perfumery and flavor compositions in the tedious work of reconstructing certain essential oils, mainly flavor oils. Its tremendous volatility and "lift" combined with effect of fresh greenness on a fruity base may give very attractive and natural aroma to the important topnotes of edible essential oils.

It is also used as a trace component of various fruit flavors. Concentration varies from 5 to 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2719.

Prod.:

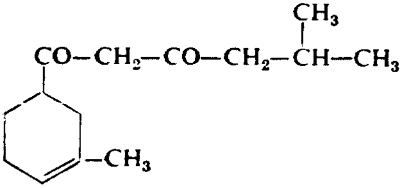
1) The *dl*-form is prepared by synthetic way.
2) The *l*-form may be prepared from Fusel amylalcohol by oxidation followed by esterification.

(66-572).

(Glidden Co., sample 1967).

## 2109: 5-METHYL-1-(3-METHYL-3-CYCLOHEXENYL)-1,3-HEXANEDIONE

The commercial product contains other isomers.



$C_{14}H_{22}O_2 = 222.33$

Colorless oily liquid or straw-colored viscous oil.

Insoluble in water, soluble in alcohol and oils.

Floral-woody odor of considerable tenacity. Variations in odor are observed in the study of materials from different suppliers.

The title ketone, which bears considerable similarity in structure to Methylionone, is a result of research on an entirely different chemical field. Many chemicals of similar structure are commercially available, mostly under trade name, however.

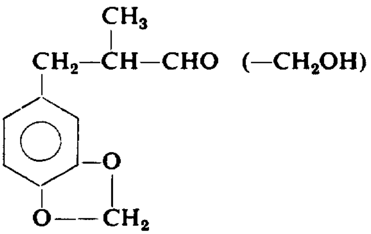
This ketone finds some use in perfume compositions, where it blends well with Styrax, Vetiver, Cedarwood derivatives, Cyclohexyl derivatives, etc. and it introduces interesting deviations from the conventional Methylionone theme.

Although the starting materials are very inexpensive commercial chemicals, the title material has not yet been offered under its proper chemical name or in a pure state as a low-cost perfume chemical.

Prod.: (several methods) e. g. from Isoprene by condensation with Methylacrylate, followed by condensation with Methyl-*iso*-butylketone. Also from *4*-Methyl-*2*-pentanone by condensation with Ethyl-*3*-methyl-*3*-cyclohexene-*1*-carboxylate.

## 2110: alpha-METHYL-3,4-METHYLENE-DIOXY HYDROCINNAMIC ALDEHYDE

"Helional" (the commercial product contains variable amounts of the corresponding alcohol).



$C_{11}H_{12}O_3 = 192.22$
(The aldehyde)

Translucent, colorless crystalline mass, or white crystalline powder. M.P. 39° C.

Sweet floral and mildly herbaceous odor of considerable tenacity. Although there is some resemblance to Heliotrope, the material also includes Anisaldehyde-like notes and power. Some perfumers find it less delicate than Heliotropine.

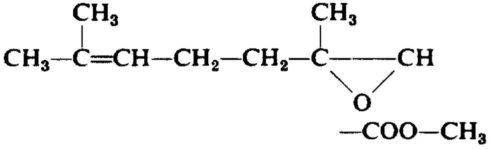
This unusual aldehyde finds limited use in perfume compositions, and it performs satisfactorily in soap, where its superior power makes it an interesting modifier for or even substitute for Heliotropine and similar floral aldehydes.

Prod.: from Heliotropine by condensation with Propionic aldehyde, followed by hydrogenation. The process results in the formation of the corresponding alcohol, which has a weaker odor but does not influence the olfactory value of the product seriously.

86-58;
(Firmenich data and sample).

## 2111: METHYL METHYLHEPTENONE GLYCIDATE

Methyl-*3,7*-dimethyl-*2,3*-epoxy-*6*-octenoate. A higher homologue of "Glycidate M-116" (two Carbon atoms higher).



$C_{11}H_{18}O_3 = 198.27$

Colorless or very pale straw-colored liquid.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils, poorly soluble in Glycerin.

Sweet caramellic-fruity and very tenacious odor. The fruity note has some resemblance to Strawberry and "cooked" Pineapple or Apricot-preserve.

Sweet and fruit-preserve-like taste in concentrations below 50 ppm.

The title material has been suggested for use in flavor compositions as a modifier for EMPG (so-called Aldehyde C-16) or as a blender-fixative in Caramel, Rum, fruit complexes, chewing gum flavors, toothpaste flavors, etc.

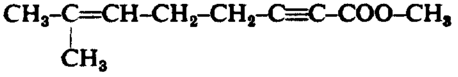
However, since the material is not specifically listed as G.R.A.S. by the American authorities, it should not be included in food flavors intended for use in the U.S.A.

Prod.: From Methylheptenone by condensation with Methyl monochloroacetate in the presence of Sodium methoxide or Sodamide.

(See also monograph: Methyl-*3,5*-dimethyl-*2,3*-epoxy-*4*-hexenoate), No. 2004.

## 2112: METHYL-6-METHYL-n-HEPT-5-EN-YNE CARBONATE

A Methyl nonenynoate.



$$CH_3\text{-}\underset{\displaystyle CH_3}{\underset{|}{C}}{=}CH\text{-}CH_2\text{-}CH_2\text{-}C{\equiv}C\text{-}COO\text{-}CH_3$$

$C_{10}H_{14}O_2 = 166.22$

Colorless oily liquid. B.P. 229° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, fatty-green, somewhat oily-waxy odor of good tenacity. The oily notes have a remote resemblance to those of Coconut meat.

This olefinic-acetylenic ester represents another type member of the great number of homologues and isomers developed in search of interesting fragrance effect. Until the appearance of a large variety of Hexenyl esters, the Acetylenic esters were among the most interesting "green" type fragrance chemicals. Most perfumers find that Amyl heptin carbonate was the most Violet-leaf-like and true-to-Nature of the series.

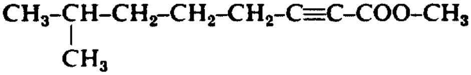
The title material is very rarely offered commercially, and it is not likely to appear in future price-lists either.

Prod.: from Methylheptenone via *6*-Methyl-*n*-hept-*5*-en-yne and its acid to the ester.

5-245;

## 2113: METHYL-6-METHYL-n-HEPT-1-YNE CARBONATE

A Methylnonynoate, an isomer of Methyl octin carbonate.



$$CH_3-\underset{\substack{|\\ CH_3}}{CH}-CH_2-CH_2-CH_2-C\equiv C-COO-CH_3$$

$C_{10}H_{16}O_2 = 168.24$

Colorless oily liquid. B.P. 216° C.

Insoluble in water, soluble in alcohol and oils.

Sharp-green, slightly oily-leafy odor of moderate tenacity. The odor is sharper, less natural and also less oily than that of Methyloctincarbonate.

It is generally considered that this ester is less interesting than its commercially available isomer, Methyloctincarbonate.

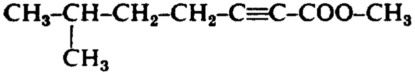
See also notes under previous two monographs.

Prod.: from Methyl-*iso*-hexylketone via *6*-Methyl-*n*-hept-*1*-yne to its acid and finally to the ester.

5-245;

## 2114: METHYL-5-METHYL-n-HEX-1-YNE CARBONATE

An isomer of Methyl heptin carbonate.
A Methyl octynoate.



$$CH_3-\underset{\substack{|\\ CH_3}}{CH}-CH_2-CH_2-C\equiv C-COO-CH_3$$

$C_9H_{14}O_2 = 154.21$

Colorless liquid. B.P. 199° C.

Insoluble in water, soluble in alcohol and oils.

Powerful "gassy"-green odor, less fatty but also less "vegetable"-like than Methyl heptin carbonate. Moderate to poor tenacity.

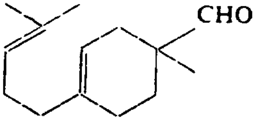
Comments on this rare acetylenic ester are much the same as for the four other branched-chain derivatives listed before and after. A possible, limited use, but no obvious advantage, and no future in perfumery.

Prod.: from Methyl-*iso*-amylketone via *5*-Methyl-*n*-hex-*1*-yne and its acid to the acetylenic ester.

5-245;

## 2115: 1-METHYL-4-(4-METHYL-3-PENTENYL)-3-CYCLOHEXENE CARBOXALDEHYDE

"Homo-Myrac aldehyde" (see Methyl pentenyl cyclohexene carboxaldehyde).



$C_{14}H_{22}O = 206.33$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, yet relatively tenacious, dry-waxy, soapy and refreshing odor, slightly camphoraceous, penetrating.

This aldehyde is occasionally offered commercially, but has found only limited use in perfumery. Those who dislike Myrac aldehyde

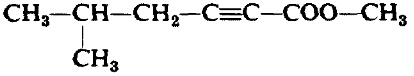
(IFF) will probably dislike this material to an even higher degree. But its power and lifting effect can be utilized with good results in Citrus compositions, and in aldehydic top-note compositions.

It gives interesting effects with the Ionones, and it is comparatively stable in soap.

Prod.: from Myrcene and Methylacrolein by condensation.

## 2116: METHYL-4-METHYL-n-PENT-1-YNE CARBONATE

A Methyl heptynoate.
An isomer of Methylhexin carbonate.



$CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-C\equiv C-COO-CH_3$

$C_8H_{12}O_2 = 140.18$

Colorless liquid. B.P. 197° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and very diffusive, "gassy"-green odor of poor tenacity. The greenness resembles that of certain Pelargonium leaves, but it is not attractive unless very highly diluted.

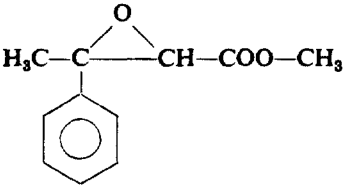
See also comments on four related acetylenic esters previous to this monograph.

Prod.: from Methyl-*iso*-butylketone via *4*-Methyl-*n*-pent-*1*-yne and its acid to the acetylenic ester.

5-245;

## 2117: METHYL METHYLPHENYL GLYCIDATE

Methylphenyl glycidic acid, Methylester.
Methyl-*alpha-beta*-epoxy-*beta*-methylhydrocinnamate.



$C_{11}H_{12}O_3 = 192.22$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sharp-fruity, pungent-sweet odor of moderate tenacity.

Sweet-fruity taste in dilutions below 20 ppm.

An absolutely Acetophenone-free grade is purely sweet-fruity at that level, while traces of Acetophenone may produce harsh notes down to a few ppm.

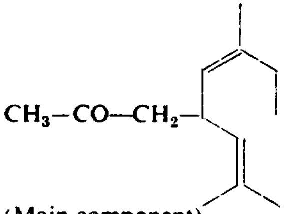
This glycidic ester finds limited use in perfumes and flavors, mainly as a modifier for the much more common Ethyl ester (see monograph). Its sweetness is not as typically Strawberry-like, but its pungency can be controlled to a point where the material lends pleasant nuances and power.

With the fruity-sweet materials often used in lipstick perfumes, it can produce pleasant variations from the stereotypical Ionone-Raspberry-Strawberry theme, particularly since many true-to-Nature and refreshing fruity items are now available.

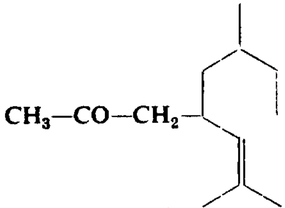
Prod.: from Acetophenone with Sodamide and Methyl monochloroacetate.

## 2118: 6-METHYL-4-(2-METHYLPROPENYL)-5-OCTEN-2-ONE

Mugylacetone.
The commercial product consists of a mixture of isomers, etc.



(Main component)



(By-component)

$C_{13}H_{22}O = 194.32$
$C_{13}H_{24}O = 196.34$

Almost colorless or pale straw-colored liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and refreshing, oily-floral and herbaceous odor of moderate tenacity. The floral notes are rose-lily-like, and the herbaceous notes blend well with Lavender or Clary Sage.

This ketone, developed parallel with the earlier and temporarily successful Geranyl acetone, has found some application in perfumes. Its power and relatively good stability in soap makes it a useful modifier for floral as well as non-floral types, or Oriental bases, etc. It blends well with Opopanax and Rose, with Lavender and Styrax, and with all the "rose alcohols" and the Linalool family.

The ketone suffers somewhat from the same disadvantage as seen in many other unsaturated ketones, a tendency to decompose, in this case a tendency to produce acetic notes. This is quite common in products made via the "enol-condensation" process.

Prod.: from Allo-Ocimenol via its chloride with Ethylacetoacetate by enol-condensation, followed by ketonic hydrolysis (decarboxylation).

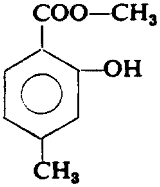
Allo-Ocimenol, commercially known as "Muguol" is a mixture of *2,6*-Dimethyl-*3,5*-octadien-*2*-ol and *3,7*-Dimethyl-*4,6*-octadien-*3*-ol (*cis*- and *trans*-isomers).

The product will also contain the ketone with only one double bond, as hydration of the Allo-ocimene yields Allo-ocimenol, commercially marketed as "Muguol".

See: *3,7*-Dimethyl-*1,6*-octadien-*3*-ol, and: *3,7*-Dimethyl-*4,6*-octadien-*3*-ol.
See also: 66-870.

## 2119: para-METHYL METHYLSALICYLATE

Methyl-*para*-methylsalicylate.
Methyl-*meta*-cresotinate.
Methyl-*2*-hydroxy-*para*-toluate.
NOTE: Do not confuse with *para*-Methoxy methylsalicylate.



$C_9H_{10}O_3 = 166.18$

Colorless liquid. Sp.Gr. 1.16. B.P. 235° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, mild, herbaceous-spicy odor, weaker than Methylsalicylate, more floral. Moderate tenacity.

Spicy-wintergreen-like taste, more floral-woody than Methylsalicylate.

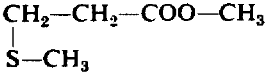
This phenolester finds a little use in perfume compositions, partly in mild or sweet leather-like notes, or in spicy floral fragrances of Tuberose-Cassie type. Its weaker odor and higher cost makes it rather uninteresting as compared to Methylsalicylate.

Prod.: by condensation of Acetoacetaldehyde with Ethylacetoacetate, followed by Methyl-esterification.

34-788; see also: 68-770;

## 2120: METHYL-beta-METHYL THIOLPROPIONATE

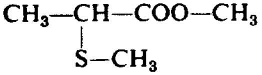
Methylmercapto methylpropionate.
*beta*-Methylthiolpropionic acid, Methylester.



$$\begin{array}{l} CH_2-CH_2-COO-CH_3 \\ | \\ S-CH_3 \end{array}$$

$C_5H_{10}O_2S = 134.20$

this material is occasionally confused with Methyl-2-methyl mercaptopropionate:



$$\begin{array}{l} CH_3-CH-COO-CH_3 \\ \quad\quad\ | \\ \quad\quad\ S-CH_3 \end{array}$$

which is an isomer of the title material.

Colorless mobile liquid. B.P. 181° C.

Very slightly soluble in water, soluble in alcohol and oils.

Extremely powerful, diffusive and penetrating sweet-sulfuraceous odor, only in dilution becoming endurable and fruity-sweet. Its Onion-like character in high concentration changes to "cooked"-fruity odor in minute concentrations.

The flavor is fruity-sweet, Pineapple-like in concentrations below 5 ppm, most pleasant below 1 ppm. The flavor is clearly perceptible and agreeable well below 0.1 ppm.

This material was synthesized shortly after being identified as a trace component in Pineapple juice in 1945. It is now used widely in Pineapple imitation flavors, and in reconstitution of Pineapple flavor in processed (canned) Pineapple preparations. Later, it has found application in meat flavors where its effect resembles that of Onion and Garlic oils: in very minute traces it simply lifts the flavor, accentuates the existing aroma without participating or contributing any typical Onion-like or other sulfuraceous flavor. The concentration used of title material is about 0.05 to 1 ppm in the consumer product.

Prod.: via Mercaptan ester reaction.

G.R.A.S. F.E.M.A. No.2720.

90-826; 140-176; 157-451; 159-663; 86-99;

## 2121: METHYL MYRISTATE

Methyl tetradecanoate.

$CH_3(CH_2)_{12}COO-CH_3$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid, or white waxy-crystalline mass, melting at 22° C. B.P. 295° C.

Insoluble in water, soluble in alcohol and oils.

Weak, oily-orrisy odor with a faint, honey-like undertone and good tenacity.

This ester finds limited use in perfume compositions, not only in Orris bases with Ionones, but also in Mimosa, Cassie, Tuberose, Honeysuckle, etc. where the effect of waxy-oily petal-notes is desirable and where a faint undertone of honeylike character may be in its place. It performs well in powder perfumes with musks and Methylionones.

The ester finds some use in flavor compositions, mainly in Honey and a few types of fruit flavor. The concentration is normally only traces, or from 0.2 to 2 ppm.

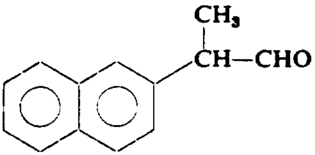
Prod.: by direct esterification of Methanol with Myristic acid under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2722.

4-93; 26-608; 86-96; 103-81; B-II-365;

## 2122: METHYL-beta-NAPHTHYL ACETALDEHYDE

*2-beta*-Naphthyl propionaldehyde.



$C_{13}H_{12}O = 182.24$

White crystals.

Practically insoluble in water, soluble in alcohol and oils.

Harsh, heavy-sweet, tenacious odor of Mandarin-Neroli type, but not as refreshing or light as Mandarin.

The title material has been suggested for use in perfume compositions, and it has been known for many decades. In spite of this, it has not achieved any world fame, and it remains unknown in many areas, nonexisting in many laboratories. The number of Naphthyl-derivatives used as floralizers in perfumery is very small, and many perfumers completely avoid the use of these materials. Others have found ways of using them with advantage, avoiding their most conspicuous drawbacks in perfumery, the appearance of "harsh" notes. Discretely used, these materials can lend enormous power at very little cost, and they are generally stable and non-discoloring.

This aldehyde is perhaps more pungent and less floral than the ethers, but it will lend power to floral compositions.

Prod.: from Propion aldehyde plus *beta*-Naphthaldehyde, followed by regulated hydrogenation.

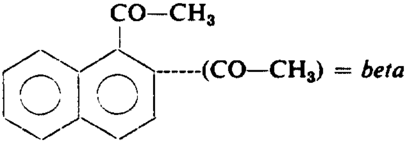
It has also been prepared from *beta*-Naphthylethanol, which may be obtained from Naphthylmagnesium bromide with Ethylene oxide.

3-82; 4-93; 7-276; 68-1326; 163-51;

## 2123: alpha-METHYL NAPHTHYL KETONE

*alpha*-Acetonaphthylene.
"Oranger liquide".
*1'*-Acetonaphtone.
"Nerolys" (also *beta*).
Anthralone.
- and many other trade names.

The commercial product is a mixture of *alpha*- and *beta*-Methylnaphthyl ketone with the former prevailing.



$C_{12}H_{10}O = 170.21$

Colorless or pale yellowish oil. B.P. 303° C. Sp.Gr. 1.12.

Insoluble in water, soluble in alcohol and oils.

Sweet, floral, but rather harsh Orange-blossom-like odor of considerable tenacity. Overall weaker than the crystalline *beta*-isomer.

This ketone has been used quite widely in perfume compositions at the time when certain processes would yield an amount of the *alpha*-isomer along with the more desirable *beta*-isomer.

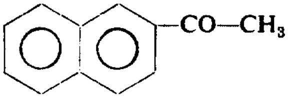
Since the cost of the liquid *alpha*-isomer is almost the same as that of the *beta*-isomer, interest has weakened much in the crude liquid, and most perfumers prefer to use only the crystalline isomer, (see next monograph).

Prod.: from Naphthalene with Acetylchloride and Aluminum chloride (Friedel-Craft's synthesis) using Carbon disulfide as solvent in order to favor formation of *alpha*-isomer.

4-93; 5-167; 86-96; 106-259;

## 2124: beta-METHYL NAPHTHYL KETONE

*beta*-Naphthyl methyl ketone.
*2'*-Acetonaphtone.
*beta*-Acetonaphthylene.
"Orenolia".
"Cetone D".
"Oranger Crystals".
Nerolys (also *alpha*-).
Nerolon.
Orangeol.
Anthralone (also *alpha*-),
– and many other trade names.



$C_{12}H_{10}O = 170.21$

White crystalline material. M.P. 55° C. B.P. 300° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and very tenacious Orangeblossom-type odor with a remotely fruity undertone.

In extreme dilution it has a Strawberry-Grape-like taste.

Overall more powerful and also more pleasant than the *alpha*-isomer. Stable in soap and most other mild alkalis. Although its odor has often been compared to that of Methyl-anthranilate, it represents an entirely different type of Orangeblossom sweetness, without the agressive harshness of the Anthranilate. Attemps have even been made to market "condensation products" of the two materials under various flowery trade names.

The material is widely used in perfume compositions, mainly in Neroli, Orangeblossom, Sweet Pea, Magnolia, Honeysuckle, Wistaria, Narcisse, Jasmin, various exotic florals such as Frangipanni, etc. It may have a perceptible effect in the perfume (or base) at concentrations well below one percent, and the effect is particularly noticeable in the terminal notes.

In flavor compositions, the ketone finds a place in imitation Strawberry, Grape, various Citrus and berry-compositions, in Neroli and other floral flavors, in fruit complexes and in certain types of Vanilla flavor. The normal concentration used will vary from 0.5 to 5 ppm, but in chewing gum it may be as high as 400 to 700 ppm.

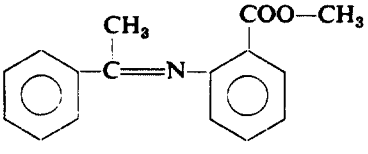
G.R.A.S. F.E.M.A. No.2723.

Prod.: from Naphthalene plus Acetylchloride and Aluminum chloride (Friedel-Craft's synthesis) in Nitrobenzene solvent.

4-93; 5-167; 86-96; 106-258; 103-273;

## 2125: METHYLNAPHTHYLKETONE-METHYLANTHRANILATE

An ill-defined product, commercially a mixture of two chemicals and an incomplete reaction product.



Theoretical structure.

$C_{20}H_{17}NO_2 = 303.36$

Very viscous yellowish or intensely yellow to pale amber-colored liquid.

Insoluble in water, soluble in alcohol and oils.

This material was obviously prepared in the hope that a combination of two well-established Orangeblossom materials would give something really outstanding. It did not. There is no indication that the title material works better in a perfume than the two parent materials separately introduced in the perfume composition. And there is no reason to go through all the trouble to make the two materials condence into one.

The material, commercially available from time to time, does have an exceptional tenacity, but so does Methyl naphthyl ketone. And the objectionable mustiness of Methyl-anthranilate is pleasantly covered by the ketone component – which it would be anyway.

Briefly, it is most conceivable that the title material will become obsolete or end up as a curiosity on the shelf.

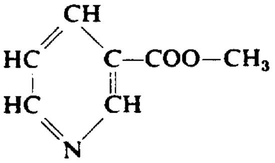
If the condensation were quantitatively complete, the title material would have the advantage of being safe against discoloration with Indole, Quinolines, etc. and there would be good reason to use such product.

Prod.: by condensation of Methylanthranilate with Methylnaphthylketone.

33-1029;
See also the individual monographs on the two parent components.

## 2126: METHYL NICOTINATE

*3*-Pyridinecarboxylic acid, Methylester.
*beta*-Pyridinecarboxylic acid, Methylester.



$C_7H_7NO_2 = 137.14$

White crystals. M.P. 39° C. B.P. 209° C.

Soluble in water, Propylene glycol, alcohol and oils.

Warm, but nauseating, sweet-herbaceous odor with mildly tobacco-like notes and moderate tenacity. In extreme dilution it displays a sweet-herbaceous, quite pleasant odor.

This ester has found limited use in perfume compositions for reasons similar to those justifying the use of Piperidine, etc. in certain floral and floral-Oriental bases, flower absolute imitations, etc.

The concentration needed should compensate for the hazards occasionally expressed in using Pyridine derivatives in perfumes. It may be interesting to note then, that Pyridine itself is permitted for use in flavor compositions in the U.S.A.

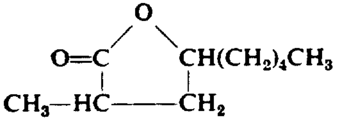
An overdose of the subject material is not very conceivable, since its effect is only pleasant at very low level. It supplies the warm and slightly nauseating-heavy, sweet-herbaceous undertone often connected with Jasmin, Tuberose, Gardenia and other heavy florals. Working with a 5 % solution of this ester, the perfumer will normally have no problem in finding the effective and pleasant level of concentration in his creation.

Prod.:
1) from Tetramethylammonium nicotinate by heating.
2) from Nicotinyl chloride hydrochloride and and Methanol in presence of Pyridine.

69-560; 100-680;

## 2127: METHYL-gamma-NONALACTONE

*alpha*-Methyl-*gamma*-amylbutyrolactone.
"*iso*-Decanolide".
*2*-Methyl-*1,4*-nonalactone.
Methyl-*gamma*-pelargolactone.



$C_{10}H_{18}O_2 = 170.25$

Colorless or pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Musty-camphoraceous, almost minty odor with only a subdued fruity undertone. Good tenacity.

In search of interesting *alpha*-alkylsubstituted *gamma*-Lactones the title material was developed, and it is mentioned in this work as a (not very successful) member of that series.

See also *delta*-Decalactone,
*gamma*-Decalactone,
*alpha*-Hexyl-*gamma*-butyrolactone.
*alpha*-*iso*-Hexyl-*gamma*-*n*-butyrolactone.

86-97;

## 2128: METHYL NONANOATE

Methyl pelargonate.
Methyl nonylate.

$CH_3{-}OOC(CH_2)_7CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 214° C.

Insoluble in water, soluble in alcohol and oils.

Fruity-winey, refreshingly Nut-Coconut-like odor of moderate tenacity.

Sweet-oily, fruity Coconut-like taste in dilutions below 10 ppm. Higher concentrations show an overpowering oily-fatty note.

This ester finds limited use in perfume compositions as part of topnotes in floral and fruity fragrance complexes. It blends well with the Citrus notes, with Neroli and Orange-blossom, with Oakmoss and Galbanum, but its power is easily underestimated.

It is more widely used in flavors, particularly in imitation Nut, Coconut, Orange, Pineapple, Honey, Cognac, Apple ("Champagne"), various fruit complexes, Citrus blends and berry flavors.

The concentration in the finished product will normally be about 3 to 7 ppm.

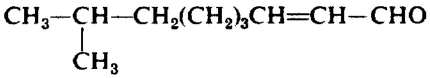
Prod.: by direct esterification of Methanol with Nonoic acid preferably using azeotropic conditions.

G.R.A.S. F.E.M.A. No.2724.

4-94; 26-610; 86-97; 103-81; 160-1140; B-II-353;

## 2129: METHYL-8-NONEN-2-AL-1

*8*-Methylnonen-*2*-al-*1*.
*3-iso*-Heptyl acrolein.



$CH_3{-}\underset{\underset{\displaystyle CH_3}{|}}{C}H{-}CH_2(CH_2)_3CH{=}CH{-}CHO$

$C_{10}H_{18}O = 154.25$

Colorless or very pale straw-colored oily liquid. B.P. 222° C. Sp.Gr. 0.85.

Fatty-citrusy, almost woody and in dilution Orange-like odor of moderate to poor tenacity. The aldehyde oxidizes easily in air and its odor is heavily influenced by such deterioration. Pronounced waxy-stearin-like or rancid notes will indicate that oxidation has already taken place. The aldehyde keeps well under Nitrogen atmosphere.

This rare aldehyde, a component of certain perfumery specialties, finds limited use in the reconstruction of certain essential oils. As part of novel topnote bases, it can introduce power and very sweet natural notes in support of Citrus oils, including Bergamot and particularly Bitter Orange.

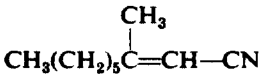
It gives interesting effects in Oriental type fragrances when Opopanax is present, or with certain herbaceous oils.

Prod.: by condensation of *iso*-Propylvaleric aldehyde (an *iso*-Octanal) and Acetaldehyde.

89-48;

## 2130: 3-METHYL-2-NONENE NITRILE

*2*-Methyl-*1*-octen-*1*-yl cyanide.
*iso*-Nonenyl cyanide.



$CH_3(CH_2)_5\overset{\overset{\displaystyle CH_3}{|}}{C}{=}CH{-}CN$

$C_{10}H_{17}N = 151.31$

Colorless or very pale straw-colored mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very powerful, dry-and-fatty, woody, Orris-like odor, in extreme dilution pleasant, fresh tobacco-like and green with some resemblance to Mimosa.

This nitrile, a relatively new development, has found a little use in perfumery as a trace ingredient along with Ionones, or as a new modifier in aldehydic-green topnote compositions, occasionally in Mimosa bases, for some inexplicable reason not very popular.

The title material has the advantages of many other Nitriles: it is quite stable under mildly alkaline conditions, and therefore recommended as a powerful ingredient in new soap fragrances. It should not be exposed to acid conditions, however, because it will break down and possibly liberate hydrocyanic acid. Normally it would produce some Methylnonenoic acid, which has an inferior odor.

See also monographs: Nonenyl nitrile and
2-Nonen-*1*-al.

Prod.: from Crotonitrile plus Hexanol.

## 2131: METHYL NONIN CARBONATE

Methyl decynoate.

$C_7H_{15}—C{\equiv}C—COO—CH_3$

$C_{11}H_{18}O_2 = 182.27$

Colorless oily liquid. B.P. 235° C.

Insoluble in water, soluble in alcohol and oils.

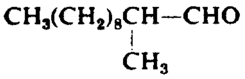
Powerful green, oily-nutty odor of moderate tenacity. The green notes are somewhat hampered by the presence of waxy-oily undertones.

This ester is probably one of the least interesting of a series of many (far too many) acetylenic esters, prepared in pursuit of the original success of Methylheptincarbonate and its nearest homologues. A few became more useful, many have lost out in competition, and they may all lose out in competition with the modern, true-to-Nature Hexenyl and Nonenyl-members.

Prod.: from *2*-Nonyne via Nonyne carboxylic acid.

## 2132: METHYL NONYL ACETALDEHYDE

*2*-Methyl undecanal.
*2*-Methylhendecanal.
"Aldehyde C-12, MNA".
"M.N.A.".
"Ambre-aldehyde".
"Ambrolene" (a stabilized solution of the aldehyde).
"*iso*-Dodecanal".
"Pekleol" (contains mainly subject aldehyde).
– and many other trade names.



$$CH_3(CH_2)_8\underset{\displaystyle CH_3}{\underset{|}{CH}}—CHO$$

$C_{12}H_{20}O = 184.32$

Colorless liquid. Sp.Gr. 0.83. B.P. 232° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, dry-Ambrelike, somewhat herbaceous odor of considerable tenacity. Although often described as "aldehydic" it has much more character than the "Lauric aldehyde" (Dodecanal). Odor descriptions of older date include the term "Orange" and this may be due to the very impure aldehyde marketed until about 1960. Up to 15 or even 20% Methyl nonyl ketone in certain commercial lots would heavily influence the refined odor of the Aldehyde.

Dry-fruity taste with Honey-Nut-like notes.

This aldehyde is probably one of the most preferred perfumery aldehydes with respect to "aldehydic topnote". It blends very well with Galbanum, the Hexenyl family or the Methyl phenyl carbinyl esters, the Methylionones or with Oakmoss. The combination of this aldehyde with Galbanum, Oakmoss and discretely fruity notes form one of the most frequently used "characters" of modern or recent perfumes, one could almost say that the theme has become "vulgarized" since it has been applied to perfumes of much lower class than where it was originally intended. It lends excellent notes to a "Tabac" base and blends well with Vetiver for such purpose. In Mimosa it will supply part of the peculiar dry notes, and in Ambre fragrances it is an almost inevitable component. Interesting effects are achieved with Ginger oil and Clary Sage.

The aldehyde finds a little use – in mere traces – in flavor compositions, mainly in Citrus complexes, Honey, Coconut, Apricot, Pineapple, etc. or in fruit blends.

The concentration will normally be about 0.1 up to 15 ppm in the finished product.

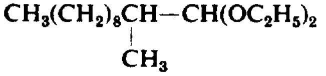
G.R.A.S. F.E.M.A. No.2749.

Prod.:

1) from Methyl nonyl ketone plus Ethyl monochloroacetate and Sodium ethylate.
2) from *alpha*-Nonyl acrolein by hydrogenation.

4-94; 5-90; 34-256; 41-36; 31-49; 86-7; 86-96; 103-188; 103-201; 106-39; 156-18; 159-408; 163-363;

## 2133: METHYL NONYL ACETALDEHYDE DIETHYLACETAL



$CH_3(CH_2)_8\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH(OC_2H_5)_2$

$C_{16}H_{34}O_2 = 258.45$

Colorless oily liquid. Sp.Gr. 0.84.
B.P. 272° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-Ambre-like, mild and semi-dry odor of mildly cinnamic-balsamic undertone and good tenacity.

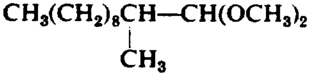
This acetal, commercially available under its proper name, has been suggested for use in perfume compositions as a support to the Aldehyde, and by itself as a novel note, applicable at much higher concentration than the Aldehyde. It introduces very pleasant tonalities with the Musks, Labdanum, Clary Sage absolute, Oakmoss and it can lift a good delicate Pine Needle fragrance out of the ordinary into the exquisite and very attractive perfumes.

Its tenacity is excellent, and with the superior stability, it should have a multitude of uses in modern perfumery.

(Sample: Haarmann & Reimer).

Prod.: by condensation of Methylnonylacetaldehyde with Ethanol.

## 2134: METHYL NONYL ACETALDEHYDE DIMETHYLACETAL



$CH_3(CH_2)_8\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH(OCH_3)_2$

$C_{14}H_{30}O_2 = 230.39$

Colorless liquid. B.P. 260° C.

Almost insoluble in water, soluble in alcohol and oils.

Refreshing and Lemony-green odor of moderate tenacity.

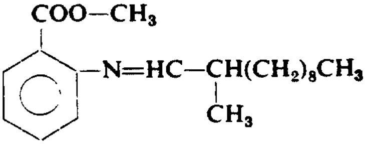
This acetal is not often offered under its proper chemical name, but it finds use as a "captive" perfume chemical in several specialties where it may form part of the topnote complex in Citrus bases, aldehydic-citrusy complexes, etc.

Prod.: by condensation of Methyl nonyl acetaldehyde with Methanol, using dry Hydrogen chloride as condensing agent.

86-96;

## 2135: METHYL NONYL ACETALDEHYDE-METHYLANTHRANILATE

(Schiff's base).
Methyl-*N*-(*2*-methylundecenylidene) anthranilate.
"Auranil MNA" (Haarmann & Reimer).



$C_{20}H_{31}NO_2 = 317.48$

Light yellow oily liquid. Sp.Gr. 0.99.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and very sweet, warm-floral and tenacious odor.

This material, of only a pale yellow color as compared to most other "Schiff's bases", has been suggested for use in perfume compositions. It is pleasantly different from most of the conventional bases, not distinctly Orange-blossom-Neroli like, but more Mandarin-Grapefruit like with almost Bitter-Orange like notes.

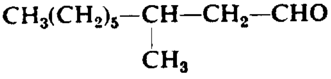
It blends very well with the Citrus oils, with the fresh-green chemicals and with Styrax, Opopanax and Patchouli in Oriental notes. For novel effects in Citrus colognes, it has endless possibilities, and it gives very attractive effects in Pine fragrances for bath preparations, etc.

(Sample: Haarmann & Reimer).

Prod.: by condensation of Methylnonylacetaldehyde with Methylanthranilate.

## 2136: 7-METHYL NONYLALDEHYDE

The title name is a commercial, but confusing name for:
*beta*-Methyl-*beta*-hexyl propionaldehyde.
More correctly called:
*3*-Methylnonanal.
*beta*-Methylnonylaldehyde.
*iso*-Decylaldehyde.
See NOTE below.



$$CH_3(CH_2)_5-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-CHO$$

$C_{10}H_{20}O = 156.27$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

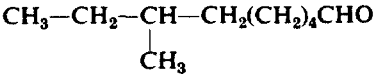
Powerful and diffusive, fresh-floral, slightly waxy odor of moderate to poor tenacity.

This aldehyde, repeatedly mentioned in perfumery literature under the name 7-Methylnonylaldehyde, has found some use in perfume compositions for its refreshing effect upon Lilac, Lily, Jasmin and many other floral fragrances. It has also good influence upon Citrus notes, sweet and bitter Orange in particular, and it gives interesting and novel notes in spicy fragrances with Bay oil or other diffusive spice odors.

Prod.: by condensation of *2*-Octanal with Acetaldehyde, followed by hydrogenation of the condensation product.

1-168; 31-49; 86-97;

NOTE: (true) 7-Methyl nonanal would normally be:

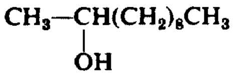


$$CH_3-CH_2-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2(CH_2)_4CHO$$

and the title material should not be confused with that aldehyde or with Methyl hexyl acetaldehyde (see that monograph) (2056).

## 2137: METHYL NONYL CARBINOL

*n*-Undecanol-*2*.
*secondary*-Undecylic alcohol.
See also monograph: Undecanol.



$$CH_3-\underset{\substack{|\\ OH}}{C}H(CH_2)_8CH_3$$

$C_{11}H_{24}O = 172.31$

Colorless viscous-oily liquid. Sp.Gr. 0.83. B.P. 233° C.

Very slightly soluble in water, soluble in alcohol and oils.

Fatty-oily-fruity odor with a relatively refreshing, almost citrusy note, distinctly different from the *primary*-Undecanol.

This alcohol finds limited use in flavor compositions, often in imitation Coconut, sometimes traces in Rum or Brandy flavors.

Its taste is more pleasant than its odor, the fatty notes apparently subdued and the fruity-nutty, sweeter notes enhanced at concentrations around 10 ppm.

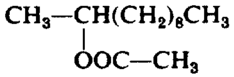
Prod.:

1) by hydrogenation of Methyl nonyl ketone (see below).
2) from Decanoic acid and Acetic acid by heating their vapors over Thorium oxide at about 450° C. The resulting ketone is subsequently hydrogenated to the alcohol.

77-172; 87-476;

## 2138: METHYL NONYL CARBINYL ACETATE

*n*-Undecanol-*2*-acetate.
*secondary*-Undecylacetate.



$$CH_3-\underset{\substack{|\\ OOC-CH_3}}{C}H(CH_2)_8CH_3$$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Oily-herbaceous, warm odor with a root-like spiciness. Odor descriptions often include the words "Gentian" and "Juniperberry", both of which point at highly attractive odor types.

This ester, not very common on the market, has found a little use in perfume compositions, particularly in support of novel topnotes in "Men's fragrances", where outdoorish, woody, spicy, herbaceous or lately Juniperberry-like notes are much in use.

The ester has also found use in Tobacco-flavorings where its warm root-like effect can be utilized with some advantage.

Prod.: by direct esterification of Methyl nonyl carbinol (see monograph) with Acetic acid, preferably under azeotropic conditions.

77-183;

## 2139: METHYL NONYLENATE

Methyl-*2*-nonenoate.
"Neo-folione" (Givaudan).
– and other trade names.

$CH_3(CH_2)_5CH{=}CH{-}COO{-}CH_3$

$C_{10}H_{18}O_2 = 170.25$

Colorless oily liquid. Sp.Gr. 0.90.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and relatively tenacious, fatty-green odor reminiscent of Violet leaf and Coconut at the same time. It is characteristic of this ester that descriptions of its odor usually start with the word "Coconut" although the material is intended to be a substitute for the acetylenic ester, Methyl heptin carbonate. However, upon dilution, the fatty-nutty notes seem to vanish and give way to a purer foliage-green odor of much softer and rounder approach than that of the acetylenic ester.

The ester finds some use in perfume compositions, not only as a Violet-leaf-like material, but also in Cucumber odors, in Ionone-rich bases as a companion to the Ionones and Methylionones, in Gardenia and other floral fragrances where a distinctly green note is desirable, and in many combinations of fruity topnotes. It is more stable than the Methyl heptin carbonate, but not quite as penetrating, gram for gram.

In flavor compositions, the material is used in Coconut, in Gooseberry and other berry imitations, in Melon flavors and many other types calling for a green note.

The concentration used is normally about 3 to 15 ppm.

G.R.A.S. F.E.M.A. No.2725.

Prod.: by Claisen condensation of Heptaldehyde and Methylacetate, using Sodium methylate condensing agent.

4-94; 7-277; 86-97; 106-275; 140-144;

## 2140: METHYL NONYL KETONE

*2*-Hendecanone.
Undecanone-*2*.
*beta*-Oxoundecane.
Nonyl methyl ketone.
M.N.K.(could refer to other perfume materials).
"Rue ketone".

$CH_3—CO—(CH_2)_8CH_3$

$C_{11}H_{22}O = 170.30$

Colorless oily liquid. Solidifies in the cold. M.P. 15° C. B.P. 225° C. Sp.Gr. 0.83.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-rosy, Orange-like odor, slightly herbaceous and orrisy in its oily notes. Poorer grades may show acrid or sharp topnotes.

Oily-fruity, also herbaceous taste with a slightly Coconut-like note.

This ketone finds very little use in perfumes as such. It has been important as starting material for the synthesis of Methyl nonyl acetaldehyde, but the synthesis is no longer entirely dependent upon this starting material.

Refreshing and powerful effects can be achieved in Lavender, Verbena and other herbaceous fragrance types, in herbal-spicy blends, in "Origan" types for novel notes, in Carnation for fruity touch to the delicate, spicy-floral notes, in Orris bases and in many types of Sweet Pea. It gives very interesting effects with Oakmoss, enhancing the non-phenolic, fresh and lifting notes in that material.

In spite of many tales of hazards of skin-irritation to this material, it is used in flavor compositions, such as Coconut, Cheese, Peach, Walnut (with Oakmoss!!), Lemon, Orange, Blackcurrant, etc.

The concentration is normally mere traces, 0.5 to 5 ppm in the finished product.

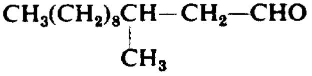
G.R.A.S. F.E.M.A. No.3093.

Prod.:
1) by oxidation of Undecanol-*2*.
2) from Decanoic acid and Acetic acid, heated over Thorium oxide to 450° C.
3) The isolation from Rue oil is of no commercial importance.

4-94; 26-608; 28-649; 31-80; 61-67; 66-516; 86-97; 89-173; 106-260; 140-165; 159-413; B-I-713;

## 2141: METHYL NONYL PROPIONIC ALDEHYDE

*beta*-Methyl nonyl propanal.
*3*-Methyl dodecanal-*1*.



$$CH_3(CH_2)_8\underset{\substack{|\\ CH_3}}{CH}—CH_2—CHO$$

$C_{13}H_{26}O = 198.35$

Colorless oily liquid.

Practically ·insoluble in water, soluble in alcohol and oils.

Waxy-fatty, "ozone"-like, in dilution very refreshing and citrusy odor of considerable tenacity.

The term "ozone"-like is rather ill-defined, but often used in describing fresh, fresh-air, outdoorish odors, not necessarily aldehydic types. Arguments are still active whether Ozone has an odor or not, whether we smell degradation products from its violent activity, or we smell the Ozone itself, etc. But the term remains in use as description for distinctly fresh outdoor odors.

This aldehyde has found limited use in perfume compositions as a modifier for Dodecanal and Methyl nonyl acetaldehyde. It resembles in odor its isomer, Tridecanal, which is also commercially available and less expensive.

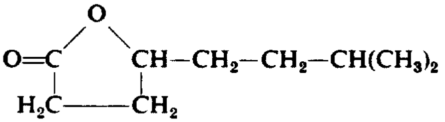
Prod.:

1) from Methyl nonyl ketone plus Ethyl monochloro propionate in presence of Sodium ethylate.
2) by hydrogenation of *beta-n*-Nonylcrotonaldehyde.

31-59; 86-97;

## 2142: 7-METHYLOCTANOLIDE-1,4

*gamma-iso*-Amyl butyrolactone.
"*iso*-Nonanolide".
See also monograph: *gamma-n*-Amyl butyrolactone. And: *alpha-iso*-Amyl-*gamma-n*-butyrolactone.



$C_9H_{16}O_2 = 156.23$

Colorless or pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-nut-like, herbaceous-musky odor of considerable tenacity. This odor complex is rather odd, and not quite as useful as that of the above mentioned isomers. The title material has been suggested for use in perfume compositions, but it is not only excessively expensive, it is also inferior in olfactory value as compared to the other members of the series. Most likely, it will vanish from the perfume laboratory shelf, if it ever reached that stage.

Prod.: from *iso*-Amyl ethylene oxide and Sodio-malonic ester.

31-174; 86-97; 156-229;

## 2143: METHYL-2-OCTENOATE

Methyl-*beta*-amylacrylate.
Methyl-2-octylenate.
*beta*-Amylpropenoic acid, methylester.

$CH_3(CH_2)_4CH{=}CH{-}COO{-}CH_3$

$C_9H_{16}O_2 = 156.23$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-green, foliage-type odor, rather sharp-green when undiluted, sweeter and more fruity when diluted below 1%. Moderate to poor tenacity.

This ester has found limited use in flavor compositions where fruity-green notes are desirable: Gooseberry, Rhubarb, Cucumber, Guava, Apple, etc.

It has been suggested for use in perfume compositions, but the author it not aware of any such use. It could probably find use as a modifier for some of the Acetylenic esters (Methyl heptincarbonate, etc.) in Narcissus, Violet and similar fragrance types.

Prod.: by direct esterification of 2-Octenoic acid and Methanol, preferably under azeotropic conditions.

140-144;

## 2144: METHYL OCTIN CARBONATE

Methyl-*2*-nonynoate.
Methyl octyne carboxylate.

$CH_3(CH_2)_5{-}C{\equiv}C{-}COO{-}CH_3$

$C_{10}H_{16}O_2 = 168.24$

Colorless oily liquid. Sp.Gr. 0.92.
B.P. 220° C.

Almost insoluble in water, soluble in alcohol and oils.

Green, Violet-leaf-like and Mimosa-like odor, more delicate and less acrid than the Methyl heptin carbonate. Moderate to poor tenacity.

In extreme dilution, pleasant, fruity-vegetable green taste, like unripe Banana, fresh Peach and Cucumber peel.

This ester finds some use in perfume compositions for its green-floral effect in Gardenia bases, Tuberose, Violet, Rose, etc. It needs considerable "frame" of supporting materials, and solid fixation, in order to behave satisfactorily. It is difficult, if not impossible, to use it as the only green material in a composition of topnote.

It blends well with fruity notes, even with heavy floral or balsamic notes, when properly toned down with equally and less volatile materials.

The ester is used in minute traces (0.02 to 10 ppm in the finished product) in imitation Peach, Banana, Cucumber, Melon, Gooseberry and other berries, fruit complexes, etc.

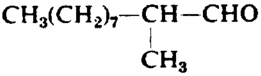
G.R.A.S. F.E.M.A. No.2726.

Prod.: from *2*-Octene via *1*-Octyne and Octyne carboxylic acid.

4-94; 5-241; 86-97; 106-261; 103-295; 156-11; 159-405;

## 2145: METHYL OCTYL ACETALDEHYDE

*2*-Methyldecanal.
"Aldehyde M.O.A."



$$CH_3(CH_2)_7{-}\underset{\displaystyle CH_3}{\underset{|}{CH}}{-}CHO$$

$C_{11}H_{22}O = 170.30$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, refreshing, dry-citrusy odor of moderate tenacity.

Less "Ambre"-like than its next higher homologue, Methyl nonyl acetaldehyde, this material offers new shades of "aldehydic" notes for variations in modern topnotes in perfumes.

It is now offered under its proper chemical name, and finds its way into several bases and perfume specialties, mainly those intended for topnote application.

It blends well with Oakmoss and Galbanum, as well as with the Citrus oils in complexes of the very popular modern type. The pronounced fruity, Orange-peel-like character of this aldehyde is particularly suitable for blending with Undecanolide, the fatty notes of which are toned down, and a pleasant freshness introduced.

Prod.: by hydrogenation of *alpha*-Octyl acrolein.

(Sample: I.F. & F.).

## 2146: METHYL OCTYL KETONE

Decanone-*2*.
Octyl methyl ketone.
Heptyl acetone.

$CH_3{-}CO{-}(CH_2)_7CH_3$

$C_{10}H_{20}O = 156.27$

Colorless oily liquid. B.P. 209° C.
Sp.Gr. 0.83. Solidifies in the cold.
M.P. 14° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, citrusy-Orange-like, peculiar floral type odor of moderate to poor tenacity.

This ketone, rarely offered under its proper chemical name, is occasionally used in perfume compositions.

It gives very interesting effects with Oakmoss, which is one of the few materials sufficiently effective as fixative for the ketone. The well-known and highly appreciated top-notes of good quality Oakmoss are enhanced and beautified by small amounts of this ketone.

It finds also limited application in flavors, particularly in imitation Coconut and Banana, where its dry-fruity character lends desirable notes.

Prod.: (many methods), e. g. by heating of vapors of Nonoic acid and Acetic acid over *Thorium oxide* at 425° C.

Also by hydrogenation of Heptylidene-acetone.

7-305; 26-608; 31-80; 45-60; 66-516; 86-97; 89-173; B-I-711; 163-59;

## 2147: METHYL OCTYL-2-OXYACETATE

Methyl octyl glycolate.

$C_8H_{17}—O—CH_2—COO—CH_3$

$C_{11}H_{22}O_3 = 202.30$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Odor of fatty alcohol, but sweet floral, less fatty and more floral than *n*-Octanol.

The taste is bitter in concentrations above 40 ppm.

This ether-ester is rarely offered commercially, and it is not likely to become a common perfumery item. Although it can be classified as "more interesting than *n*-Octanol", there is not much interest in that alcohol in the first place, and any substitute would have to be not only better but also equal in cost.

Prod.: (several methods) e. g. from *n*-Octanol plus Methyl diazoacetate.

31-158;
See also: Ethyl octyl-*2*-oxyacetate.

## 2148: METHYL-3-OCTYNOATE

An isomer of Methyl heptin carbonate.

$CH_3(CH_2)_3{\equiv}C—CH_2—COO—CH_3$

$C_9H_{14}O_2 = 154.21$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful green odor of fresh-cut grass type, but with pronounced fatty notes.

This ester was prepared along with a great number of isomers and homologues in search of more interesting members of the Acetylenic ester family.

However, it failed to interest the perfumers and it appears to have fallen into oblivion on the research shelf. In view of the rapid development in the field of new natural green odors in the past decade, it is most conceivable that the Acetylenic esters, even those of previously established interest, will become obsolete.

See also the following four isomers.

86-97;

## 2149: METHYL-4-OCTYNOATE

An isomer of Methyl heptin carbonate.

$CH_3(CH_2)_2C{\equiv}C(CH_2)_2COO—CH_3$

$C_9H_{14}O_2 = 154.21$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful green-vegetable, Cucumber-like odor with a fruity-juicy undertone.

This isomer is probably the most interesting and pleasant next to the commercial Methylheptincarbonate. It is even less fatty and has a fresher, more vegetable-green odor.

The reason for its absence from the market may be found in troublesome preparation and a cost which cannot compete with that of the Methyl-*2*-octynoate.

See also notes under previous monograph.

See the three following monographs on isomers.

86-97;

## 2150: METHYL-5-OCTYNOATE

An isomer of Methyl heptin carbonate.

$CH_3{-}CH_2{-}C{\equiv}C(CH_2)_3COO{-}CH_3$

$C_9H_{14}O_2 = 154.21$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-green, Violet-leaf and Cucumber peel type odor of moderate to poor tenacity.

Except for its inferior power, this isomer could be the most interesting of all the Methyl-heptincarbonates. But it is rarely seen on the market, and it may never become a standard item on the perfumer's shelf.

See notes under Methyl-*3*-octynoate.

See also the following two monographs.

86-97;

## 2151: METHYL-6-OCTYNOATE

An isomer of Methyl heptin carbonate.

$CH_3{-}C{\equiv}C(CH_2)_4COO{-}CH_3$

$C_9H_{14}O_2 = 154.21$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Bitter-green, earthy-green, Reseda-like odor of moderate to poor tenacity.

This isomer is rather uninteresting but is mentioned mainly for the sake of completing the series of monographs on the Methyl heptin carbonates.

See notes under monograph: Methyl-*3*-octynoate.

See also following monograph.

86-97;

## 2152: METHYL-7-OCTYNOATE

An isomer of Methyl heptin carbonate.

$CH{\equiv}C(CH_2)_5COO{-}CH_3$

$C_9H_{14}O_2 = 154.21$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and intensely green odor, but rather fatty and not typical of Violetleaf, nor is it reminiscent of any distinct natural material.

This isomer is not too interesting, and the author is inclined to believe, that apart from the well-established Methyl-*2*-octynoate (commercial Methyl heptin carbonate), only the *4*- and the *5*-isomers could have become items of commercial interest.

The availability of many naturally occurring and highly interesting Hexenyl derivatives and members of the Nonenal and Nonadienol families will most conceivably steal all the interest away from the Acetylenic esters.

See the four preceding monographs.

86-97;
Also: Journal of American Chemical Society 71, 1292 (1949).

## 2153: METHYL OLEATE

*cis*-Methyl-9-octadecenoate.

$CH_3(CH_2)_7CH{=}CH(CH_2)_7COO{-}CH_3$

$C_{19}H_{36}O_2 = 296.50$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. higher than 300° C.

After storage, often a pale yellowish oil.

Insoluble in water, soluble in alcohol and oils.

Mild-fatty, oily odor of considerable tenacity. The oily notes are pleasant, natural and not rancid (unless material is over-aged or improperly stored).

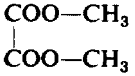
This ester finds some use in perfume compositions, mainly in certain flower bases and floral compositions, calling for oily notes in the floral, petal-like portion of the odor. Jasmin, Tuberose, Gardenia and several other floral bases may benefit from the effect of this ester, although many related materials are used for the same purpose.

Prod.: by direct esterification of Methanol with Oleic acid, e. g. under azeotropic conditions.

4-94; 26-608; 160-1132; B-II-467;

## 2154: METHYL OXALATE

Dimethyl oxalate.
Dimethylethane dioate.



$$\begin{array}{l} COO{-}CH_3 \\ | \\ COO{-}CH_3 \end{array}$$

$C_4H_6O_4 = 118.09$

Colorless monoclinic tabloid crystals.
M.P. 54° C. B.P. 164° C. Sp.Gr. 1.15 (liquid).

6% soluble in water (but hydrolyzes easily). Soluble in alcohol and oils.

Although virtually odorless, this ester has occasionally been used in perfumes for its peculiar "lifting" effect which is *not* accompanied by an additional odor or perceptible note. One could almost classify the effect as "anti-fixative". However, the poor stability of this material in presence of water (moisture) is a serious drawback.

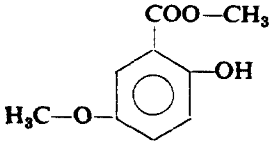
Oxalic acid as such is occasionally used to remove iron from certain essential oils in order to lighten their color (Patchouli, Vetiver, etc.) but it is generally considered an undesirable material in perfumes.

Prod.: by azeotropic type esterification of Methanol with Oxalic acid.

4-94; 26-518; 66-956; 100-680; 160-1134; B-II-534;

## 2155: METHYL-2-OXY-5-METHOXYBENZOATE

5-Methoxy methylsalicylate.
Methylgentisate-5-methylether.



$C_9H_{10}O_4 = 182.18$

Colorless oily liquid. B.P. 255° C.

Slightly soluble in water, soluble in alcohol and oils.

Warm, woody-herbaceous and quite tenacious odor.

This Phenol-ether-ester has been suggested for use in perfume compositions where it can add very pleasant tonalities in combination with Oakmoss and Vetiver. It blends generally well with herbaceous notes, and its sweet-rooty odor can be utilized in novel Oriental type fragrances. It is supported well by

Coumarin derivatives, but it carries the disadvantages of being a Phenol, sensitive to alkali and iron.

Prod.:

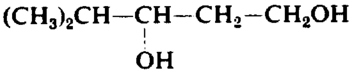
1) (natural) by hydrolysis of Primulaverin, the glycoside of Primrose rhizomes.
2) from Salicylic acid by oxidation with Potassium persulfate and Ferrous sulfate. Then alkaline methylation, followed by esterification.

See also: *para*-Methoxy methylsalicylate.

68-567; 68-777;

## 2156: 5-METHYL-1,3-PENTANEDIOL

Methyl-*beta*-pentylene glycol.



$(CH_3)_2CH-\underset{OH}{\underset{|}{CH}}-CH_2-CH_2OH$

$C_6H_{14}O_2 = 118.18$

Colorless, slightly oily-viscous liquid.

Sp.Gr. 0.92. B.P. 197° C.

Faint, musty and not very pleasant odor (commercial grade material).

This glycol is probably not used in perfumes or flavors as an active olfactory ingredient. It is briefly mentioned in this work in order to elucidate a problem of possible confusion with:

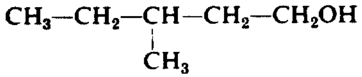
*2*-Methyl-*2,4*-pentanediol, which is commercially known as Hexylene glycol, and recommended for use as a solvent in flavors. It is also used as a solvent in certain types of perfume. It has a faint odor (musty), a bitter taste in concentrations higher than 20 ppm, and it is miscible with water, alcohol and many oils, including some Citrus oils. It is not a good solvent for Monoterpenes.

The title material is used as parent component in a series of reactions aimed at preparing new ketals. Even more interesting are the ketals made from *2,2*-Dimethyl-*1,3*-propanediol.

(Union Carbide Chemical Co. data – on Hexylene glycol).

## 2157: d-3-METHYLPENTANOL-1.

*3*-Methyl-*1*-pentanol.
*active*-Hexylalcohol.



$CH_3-CH_2-\underset{CH_3}{\underset{|}{CH}}-CH_2-CH_2OH$

$C_6H_{14}O = 102.18$

Colorless liquid. Sp.Gr. 0.83. B.P. 154° C.

Insoluble in water, soluble in alcohol and oils.

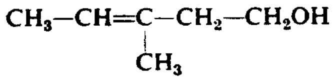
Vinous, earthy-green odor, giving a "bitter" odor impression, sometimes referred to as "metallic". Moderate to poor tenacity.

This alcohol finds limited use in perfumery, mainly as a component of artificial Geranium oil, etc.

26-574; 87-467; 160-1144; B-I-411;

## 2158: 3-METHYL-3-PENTEN-1-OL

Methyl pentenol.



$CH_3-CH=\underset{CH_3}{\underset{|}{C}}-CH_2-CH_2OH$

$C_6H_{12}O = 100.16$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, fruity-green, leafy, Geranium-green type odor of poor tenacity.

This alcohol has been suggested for use in perfume compositions, originally as part of the earthy-green complex of Geranium oil (artificial). However, it does not seem to lend the same natural tonalities as those obtained with *2*-Hexenol or *3*-Hexenol.

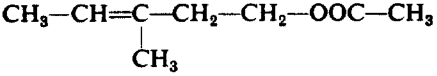
The alcohol is still used to a minor extent in certain topnotes and it performs quite pleasantly with Galbanum and the Methyl phenyl carbinyl esters.

Prod.: from Acetylene via Methylpentynol, followed by hydrogenation. (Hoffmann-laRoche).

*2*-Methyl-*4*-penten-*2*-ol is also known (produced from Allyl magnesium bromide plus Acetone by Grignard type reaction).

## 2159: METHYL PENTENYL ACETATE

*3*-Methyl-*3*-penten-*1*-yl acetate.



$CH_3{-}CH{=}\underset{\overset{|}{CH_3}}{C}{-}CH_2{-}CH_2{-}OOC{-}CH_3$

$C_8H_{14}O_2 = 142.20$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very diffusive, fruity-green, Banana-like odor. Overall much fresher than Amylacetate, and somewhat similar to Prenyl acetate.

Moderate to poor tenacity.

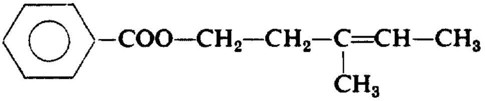
This ester has been suggested for use in perfume compositions as part of modern topnotes, where fruity and green odors may be combined to produce or imitate topnotes of very well known market perfumes.

The title ester introduces freshness and "lift" to herbaceous fragrance types, and brings "life" into Lavender and similar types. It has also found some use in combination with Lavandin oil for soap.

Prod.: by azeotropic type esterification of the alcohol (see previous monograph) with Acetic acid.

## 2160: METHYL PENTENYL BENZOATE

*3*-Methyl-*3*-penten-*1*-yl benzoate.



$C_{13}H_{16}O_2 = 204.27$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-fruity, slightly green and floral odor of fair to good tenacity.

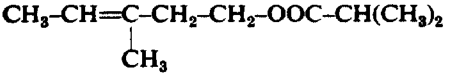
This ester, a member of a long series of esters of Methylpentenol, has been suggested for use in perfume compositions, particularly as a modifier in Fougères, where it may introduce interesting new notes, and in Oriental fragrance types, Mimosa notes, etc.

It does not seem to have caught the interest of the perfumers, and chances are that it will never become a very common perfume chemical, since it has been available for almost 10 years and not yet come into strong demand.

Prod.: by azeotropic type esterification of Methylpentenol with Benzoic acid.

## 2161: METHYL PENTENYL-iso-BUTYRATE

*3*-Methyl-*3*-penten-*1*-yl-*iso*-butyrate.



$CH_3{-}CH{=}\underset{\overset{|}{CH_3}}{C}{-}CH_2{-}CH_2{-}OOC{-}CH(CH_3)_2$

$C_{10}H_{18}O_2 = 170.25$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-fruity, Pear-like odor of moderate tenacity.

This ester has been suggested for use in

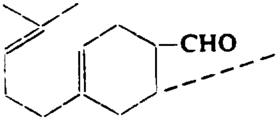
perfume compositions, where it can add power and freshness to Bergamot and Lavender notes, support Linalyl esters, and add sweetness to herbaceous and citrusy fragrance types.

This and other members of the Methylpentenyl series are not extremely popular and seem to lose ground in the competition with the now freely available *2*-Hexenylesters, and to some extent, the *3*-Hexenylesters.

Prod.: by azeotropic type esterification of Methylpentenol with Butyric acid.

## 2162: 4-(4-METHYL-3-PENTEN-1-YL)-3-CYCLOHEXENE-1-CARBOXALDEHYDE

*iso*-Hexenyl cyclohexene carboxaldehyde.
*iso*-Hexenyl tetrahydrobenzaldehyde.
"Myrac aldehyde" (I.F. & F.).
"Citrial" (Stepan-Maywood).
"Hesperia".
"Reyn-o-miral".
– and many other trade names.



(Commercial product usually contains some *meta*-isomer).

$C_{13}H_{20}O = 192.30$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and penetrating, waxy-citrusy, in dilution fresh-floral, clean and light odor with some resemblance to Dodecanal, Cyclamal and Myristic aldehyde.

Waxy-slightly bitter taste in concentrations higher than 10 ppm, overall a rather unpleasant taste.

This aldehyde, marketed several decades ago, has taken a long time to become popular, and it is questionable if one can make that statement even today. It is beyond doubt, that the aldehyde has an excellent influence upon Bergamot and other citrusy odors, and that its effect includes the "aldehydic" topnote effect to a certain degree. It performs well in soap and adds freshness to a wide range of odor types from Pine needle to Muguet, from Violet to Lilac, etc. Its very low cost makes it a candidate for industrial masking, detergent fragrances and many other large-volume products. It blends well with Ionones and the Cedarwood-like Cyclohexane derivatives in modern soap odors.

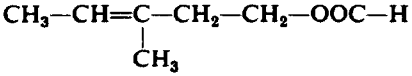
Prod.: originally developed from chemical research on insect repellants, this aldehyde is prepared from Myrcene and Acrolein.

The next higher homologue (prepared from Methyl acrolein is mentioned in this work under: Methyl-methylpentenyl-cyclo-hexene-carboxaldehyde.

The hydroxylated aldehyde, known under the name "Lyral", is listed in this work as Hydroxymethyl-pentyl-cyclohexene-carboxaldehyde. It is far more successful than the title aldehyde, but it is in no way olfactorily related to it. (See 1754).

## 2163: METHYL PENTENYL FORMATE

*3*-Methyl-*3*-penten-*1*-yl formate.



$$CH_3{-}CH{=}\underset{\displaystyle CH_3}{\underset{|}{C}}{-}CH_2{-}CH_2{-}OOC{-}H$$

$C_7H_{12}O_2 = 128.17$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-leafy, citrusy-green, dry-fruity and very diffusive odor of poor tenacity.

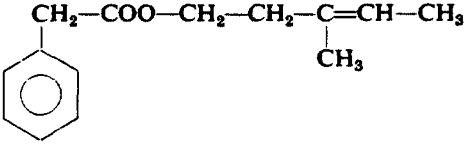
This ester has been suggested for use in perfume compositions, mainly as part of very light topnotes, modern fruity-green notes, etc. in herbaceous and light-floral fragrance types.

Although it is fairly stable under normal end-use conditions, it has failed to catch the interest of perfumers, who may have been overwhelmed with "green" materials during the past decade or so.

Prod.: by formylation of Methyl pentenol.

## 2164: METHYL PENTENYL PHENYLACETATE

*3*-Methyl-*3*-penten-*1*-yl phenylacetate.



$C_{14}H_{18}O_2 = 218.30$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful green-floral, heavy and sweet odor of considerable tenacity.

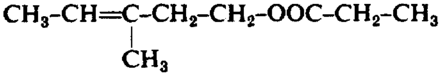
This ester finds limited use in perfume compositions as a modifier in Muguet, Gardenia, Tuberose, Hyacinth and other floral and floral-green bases. It blends well with the floral-green carbinols (in Muguet) and with Cinnamic derivatives (in Hyacinth) or the Methylphenylcarbinylesters in Gardenia.

It is interesting to note that it is quite different from the two commercially available Hexenyl phenylacetates, one of which is also found in Nature.

Prod.: by azeotropic type esterification of Methyl pentenol with Phenylacetic acid.

## 2165: METHYL PENTENYL PROPIONATE

*3*-Methyl-*3*-penten-*1*-yl propionate.



$$\mathrm{CH_3{-}CH{=}\underset{\displaystyle CH_3}{\underset{|}{C}}{-}CH_2{-}CH_2{-}OOC{-}CH_2{-}CH_3}$$

$C_9H_{16}O_2 = 156.23$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

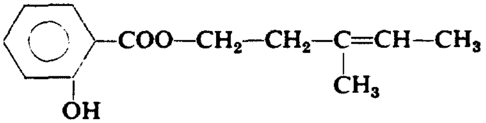
Fruity-sweet, powerful odor of moderate to poor tenacity.

Its fruity notes are rather nondescript, and this may partly count for the fact that this ester has not become very popular. It could find some use in perfume compositions as a "lifting" agent in Lavender and Bergamot compositions, a freshener in citrusy or fruity topnotes, and in general as a powerful, light ingredient in Citrus-colognes, etc.

Prod.: by azeotropic type esterification of Methyl pentenol with Propionic acid.

## 2166: METHYL PENTENYL SALICYLATE

*3*-Methyl-*3*-penten-*1*-yl salicylate.



$C_{13}H_{16}O_3 = 220.27$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet, slightly green-fruity odor with a minty undertone.

Good tenacity.

This ester, like the previously mentioned six esters of same alcohol, was developed at a time when the corresponding *2*-Hexenyl- and *3*-Hexenyl esters were not yet commercially available, or available on a limited scale only. It is quite possible that if the Methylpentenyl esters had appeared still another decade earlier, they could have become quite popular items and be firmly established in many formulae today.

But as an overall picture, they do not compete favourably with the more natural smelling Hexenylesters, and the title ester is no exception.

In view of its much lower cost, it could still find some use in novel Fougère types, herbaceous fragrances and certain fantasy perfumes.

Prod.: by azeotropic type esterification of Methylpentenol with Salicylic acid.

## 2167: METHYL-n-PENTIN CARBONATE

Methyl pentyne carbonate.
Methyl hexynoate.

$$CH_3—CH_2—CH_2—C≡C—COO—CH_3$$

$C_7H_{10}O_2 = 126.16$

Colorless mobile liquid. B.P. 171° C.

Almost insoluble in water, soluble in alcohol and oils.

Very diffusive, sharp-green and in high concentration "gassy" odor of poor tenacity. Leafy-green, but still somewhat "metallic" in dilution.

The comments made for five other acetylenic esters earlier in this work also apply to the subject ester. Not nearly as versatile as the Hexenyl esters, and not nearly as natural in its tonalities.

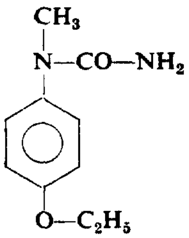
Rarely offered commercially, and probably becoming obsolete within the next decade or so.

Prod.: from Methyl propyl ketone via *n*-Pent-*1*-yne and its acid to the acetylenic ester.

5-245;

## 2168: N-METHYL PHENETHYL CARBAMIDE

*N*-(*para*-Ethoxyphenyl)-*N*-methylurea.
Methyl phenethyl urea.
"Homo-dulcin".



$C_{10}H_{14}N_2O_2 = 194.24$

Odorless crystals.
22% soluble in water at room temperature. Slightly soluble in alcohol, poorly soluble in oils.

Intensely sweet taste, but pronounced bitter aftertaste. In this respect it is poorer than Dulcin, the next lower homologue.

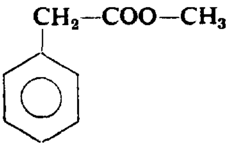
This material was developed in search of sweetening agents comparable to Dulcin, but possessing a better solubility in water. The title material is much more soluble (Dulcin is only about 0.1% soluble in cold water), and the "Homo-dulcin" is approximately 200 times sweeter than cane sugar, which is slightly inferior to the effect of Dulcin.

In view of the 1950-banning by the FDA of Dulcin as a sweetening agent, it is most conceivable that the subject material should be omitted from food. It is mentioned in this work mainly for the completion of monographs on sweetening agents.

30-336; 159-523;

## 2169: METHYL PHENYL ACETATE

Methyl-*alpha*-toluate.



$C_9H_{10}O_2 = 150.18$

Colorless liquid. Sp.Gr. 1.07. B.P. 220° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and quite diffusive honey-musky odor with traces of Jasmin-floral notes and moderate to poor tenacity.

Fruity-honey-like, very sweet taste in dilutions below 50 ppm.

This ester is widely used in perfume compositions, partly on account of its power and very low cost, partly because of its versatility in combining with floral and non-floral, particularly "Oriental" type fragrance materials. Although mainly a "topnote" material, it can easily be withheld by fixatives, musks in particular, to produce intensely sweet undertones of lasting effect. However, if it contains more than minute traces of Phenylacetic acid, the material may easily surprise the perfumer with an exceptionally tenacious and not always desirable animal, rather unclean undertone.

The ester finds use in inexpensive types of Rose, a classical ingredient in the "Rose Eglantine" type, particularly for detergent perfumes, household odors, etc. It has excellent masking effect upon the solvents used in floor waxes and furniture waxes, and its honey-like odor fits well into wax products.

Used with extreme discretion in combination with Indole, it can give suitable Civet-like effects for Jasmin and Rose fragrances, or for Oriental notes.

In flavors, it has found a major field of application in Tobacco flavoring, but mostly for the "Oriental" type of tobacco. Traces are used in imitation Strawberry, Peach and Chocolate, while it may be a larger ingredient in Honey flavors.

The concentration used may vary from 0.1 to 35 ppm in the finished product.

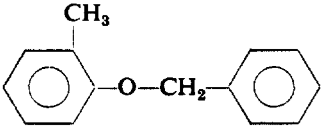
G.R.A.S. F.E.M.A. No.2733.

Prod.: from Benzyl cyanide by acid hydrolysis in presence of Methanol. Benzyl cyanide (the Nitrile of Phenylacetic acid) is derived from Benzyl chloride, an industrial chemical.

4-94; 26-610; 34-245; 68-595; 77-194; 86-98; 95-185; 96-210; 106-262; 140-151; 160-1256; B-IX-434;

## 2170: 2-METHYL PHENYL BENZYLETHER

Methyl phenyl benzyloxide.
Benzyl tolylether.
Tolyl benzyl ether.
(An isomer of *ortho*-Cresylether).



$C_{14}H_{14}O = 188.28$

White or colorless crystals. Impure commercial grades may be oily colorless liquids.

Insoluble in water, soluble in alcohol and oils.

Somewhat gassy-Geranium-like odor, in high concentrations rather unpleasant, almost Leek-like in pungent vegetable notes, but in proper dilution more green-herbaceous, yet still "acetylenic" in its overall type.

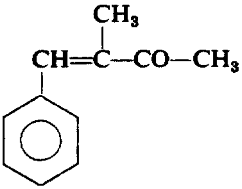
Has been suggested for use as a fixative in floral fragrances, but is rarely offered commercially, and does not offer any outstanding effects to the perfumer.

Prod.: from Benzylchloride plus *ortho*-Cresol in aqueous alkaline solution.

4-95; 31-146;

## 2171: 3-METHYL-4-PHENYL-3-BUTEN-2-ONE

Benzylidene methyl ethyl ketone.
*alpha*-Methylcinnalylidene methylketone.
Benzylidene acetone methyl.
*alpha*-Methyl-*alpha*-benzalacetone.
"Malvone" (Agfa).
"Lavandozon" (Haarmann & Reimer).



$C_{11}H_{12}O = 160.22$

Pale yellowish crystals.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, fruity-caramellic, berry-like odor of good tenacity.

The effect is overall milder than that of Benzylidene acetone.

Sweet fruity, Cherry-Plum-like taste in dilutions below 10 ppm. Somewhat bitter at higher concentrations.

Trace amounts give interesting effects in Lavender fragrances.

This ketone finds some use in flavor compositions, although there are several chemicals of similar and better type available. Traces are used in many berry compositions, imitation Cherry, Vanilla and in Nut complexes.

The concentration will normally be as low as 0.5 to 3 ppm in the finished product.

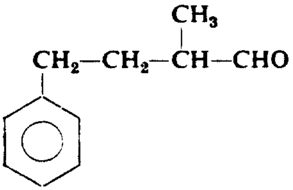
Prod.: by condensation of Benzaldehyde with Methyl ethyl ketone.

G.R.A.S. F.E.M.A. No.2734.

86-89; 4-19;

## 2172: 2-METHYL-4-PHENYL BUTYRALDEHYDE

*alpha*-Methyl-*gamma*-phenylbutanal.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Earthy-musty, but sweet and also floral, quite tenacious odor of Lilac-Hyacinth type, but less floral than Hydratropic aldehyde.

Sweet, slightly fruity and Nut-like taste in dilutions below 5 ppm. The effect resembles to some degree that of Hydratropic aldehyde dimethylacetal.

This aldehyde finds limited use in flavor compositions, particularly in Nut and Raspberry. In the latter flavor type, it may introduce the "seed-like" effect, sometimes achieved with Hydratropic aldehyde dimethylacetal.

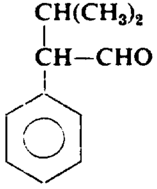
Prod.:

1) from Propion aldehyde plus Phenylacetaldehyde by condensation, followed by regulated hydrogenation.
2) by rearrangement of *2*-Methyl-*2*-phenylbutanediol.

G.R.A.S. F.E.M.A. No.2737.

## 2173: 3-METHYL-2-PHENYLBUTYRALDEHYDE

*alpha-iso*-Propyl phenylacetaldehyde.
(An isomer of "Cortexal").



$C_{11}H_{14}O = 162.23$

Colorless oily liquid. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Green-fruity, in dilution sweet and moderately tenacious odor.

In concentrations below 5 ppm the taste is rather fruity. At higher levels, it is greener, more floral and bitter at concentrations above 20 ppm.

This aldehyde is used to a minor degree in fruit flavors. The concentration is rarely higher than 1 ppm, normally between 0.1 and 0.5 ppm calculated in the finished product.

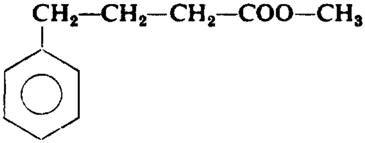
G.R.A.S. F.E.M.A. No.2738.

Prod.:

1) from Phenyl-*iso*-propylglycidic acid.
2) by rearrangement of *2*-Phenylpentane-*1,2*-diol.

## 2174: METHYL PHENYLBUTYRATE

Methyl-*4*-phenylbutyrate.
*gamma*-Phenylbutyric acid, Methylester.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol, miscible with oils.

Powerful, sweet-fruity, honey-floral odor of moderate to good tenacity.

Intensely sweet, slightly fruity taste, pleasant only in concentrations below 10 ppm. Honey-like taste appears also below that concentration, while the fruity taste turns Strawberry-like at extremely low concentration only.

This comparatively rare ester finds some use in flavor compositions, mainly as a modifier in Strawberry imitation, where is seems to do a better job, although perhaps not with the same power – as Methyl cinnamate and Methyl-hydrocinnamate (the next lower homologue to the title material). It is also used in trace amounts in Honey imitations and in various fruit complexes.

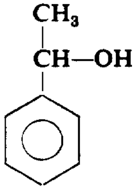
Concentrations are usually about 0.5 to 1.5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2739.

Prod.: by direct esterification of *gamma*-Phenylbutyric acid, which may be obtained from Benzoyl propionic acid by Clemmensen type reduction.

## 2175: METHYL PHENYL CARBINOL

*alpha*-Methyl benzylalcohol.
*alpha*-Phenylethylalcohol.
*1*-Phenylethan-*1*-ol.
"Styrallyl alcohol".
"Styrolyl alcohol".
Phenyl methyl carbinol.



$C_8H_{10}O = 122.17$

Colorless liquid. Sp.Gr. 1.01. B.P. 204° C. Solidifies in the cold (when it is a good, pure grade) and melts again at about 20° C.

Almost insoluble in water, miscible with alcohol and oils.

Dry-floral, earthy-green, Lilac-Jasmin-Mimosa type odor of moderate to poor tenacity. Commercial grades may carry a perceptible note of Acetophenone.

Green-fruity taste in dilutions below 10 ppm. Rather harsh and unnatural effect at higher levels.

This alcohol, an isomer of the widely used Phenylethylalcohol, finds only limited use as such in perfumes. Its esters (see the following 13 monographs) are often better known, the acetate in particular a commonly used perfume material.

The alcohol itself may lend the appropriate dry notes to a Lilac, or the earthy-woody and delicate green notes to a Mimosa, but it fails to provide a generally acceptable and versatile foundation for any type of perfume. It must be admitted, that among the reasons for its limited use is the fact that it appears on the market in an unsatisfactorily purified grade. A truly pure, olfactorily pure, Methylphenylcarbinol, provides very pleasant and soft notes for Narcissus, Violet, Honeysuckle and a multitude of florals and semi-florals, as well as Oriental and Chypre-type fragrances.

The alcohol is also used in flavor compositions, such as imitation Strawberry, Honey, and in various fruit complexes or in Oriental

Rose flavors. The concentration used is normally about 1 to 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2685.

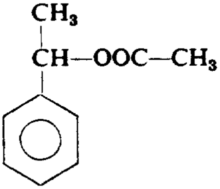
Prod.:

1) by hydrogenation or reduction of Acetophenone (commercial grade).
2) from Methyl magnesium chloride plus Benzaldehyde by Grignard type reaction. This may yield olfactorily pure material.

4-95; 5-67; 26-654; 31-23; 34-162; 65-87; 68-499; 85-87; 86-98; 103-291; 106-263; 156-75; 160-866; B-VI-475;

## 2176: METHYL PHENYL CARBINYL ACETATE

Phenyl methyl carbinyl acetate.
*alpha*-Methyl benzyl acetate.
"Phenylethylene acetate".
*alpha*-Phenylethyl acetate.
*secondary*-Phenylethyl acetate.
"Gardenol".
"Gardeniol II".
"Styrolene Acetate" (name also used for Phenylethyleneglycol monoaceatate).
"Styrallyl acetate".



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid. Sp.Gr. 1.03. B.P. 214° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and penetrating, green-floral, in dilution more fruity odor of moderate to poor tenacity.

Peculiar tart-fruity, green berry-fruity taste in dilutions below 20 ppm.

This ester is very widely used in perfumery and constitutes part of the topnote of several very successful and well-known perfumes.

It is conventionally classified as a Gardenia-green material, but its odor is typical only of certain stages of maturity of the Gardenia flower, and only of certain species. However, the ester finds use in numerous fragrance types, mostly those including fruity and green notes, and it plays an important role in topnote complexes including Oakmoss, Galbanum, Allyl ionone, Citrus oils, etc. In spite of its apparent harshness, it can be applied at comparatively high concentration, often exceeding 2 or 3%. If Benzylacetate and Citrus oils are present, the level of the title ester can be still higher. Care should be taken in evaluating the effect of this material too quickly. It will characteristically "mellow-in" the perfume composition very perceptibly after 24 hours, often more in several days or so.

Smaller amounts are used in Lilac, Hyacinth, Tuberose, Muguet, etc.

The ester finds extensive use in flavor compositions, particularly the "sharp"-fruity types, Pineapple, Apricot, Gooseberry, Apple, but also in Plum, Peach and many berry or fruit complexes.

The concentration is about 1 to 30 ppm in the finished product.

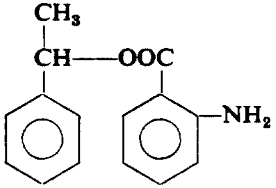
G.R.A.S. F.E.M.A. No.2684.

Prod.: by direct esterification of Methyl phenyl carbinol with Acetic acid under azeotropic conditions.

5-68; 7-340; 8-112; 33-502; 34-162; 86-98; 90-335; 103-292; 106-264; 140-137; 4-95;

## 2177: METHYL PHENYL CARBINYL ANTHRANILATE

"Styrallyl anthranilate".
*alpha*-Methylbenzyl-*ortho*-aminobenzoate.



$C_{15}H_{15}NO_2 = 241.29$

Colorless or pale straw-colored oily liquid, solidifying in the cold.

Practically insoluble in water, soluble in alcohol and oils.

Samples from different sources show such difference in odor characteristics, that one is tempted to claim that the absolutely pure material is virtually odorless. Commercial grades display variable amounts of Orange-blossom or Lilac or Narcisse-type odor, depending upon the method of production and of purity of the resulting ester.

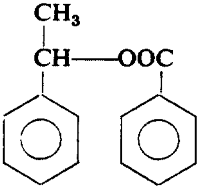
Perfumers have probably been annoyed with the variations in odor when evaluating samples of this item, and there is not much interest in the ester. It could find some use as a fixative since its effect is quite apparent when it is mixed with lower boiling odorant chemicals. It can give useful effects in Honeysuckle, Sweet Pea and other sweet florals, and its tenacity is excellent.

Prod.: from Isatoic anhydride and Methyl phenyl carbinol.

34-1012; 103-292;

## 2178: METHYL PHENYL CARBINYL BENZOATE

*alpha*-Methyl benzyl benzoate.
"Styrallyl benzoate".



$C_{15}H_{14}O_2 = 226.28$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Practically odorless when pure. However, when incorporated in floral or Oriental fragrance types, the subject material does lend a perceptible effect beyond that of fixation.

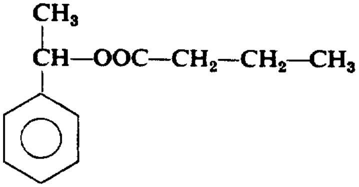
Lilac, Lily, Hyacinth and certain types of Rose may benefit from the delicate softness supplied by this tenacious material.

Prod.: by direct esterification of Methyl phenyl carbinol with Benzoic acid under azeotropic conditions.

103-292;

## 2179: METHYL PHENYL CARBINYL-n-BUTYRATE

*alpha*-Methylbenzyl-*n*-butyrate.
"Styrallyl butyrate".



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar fruity-floral odor with Jasmin-like notes. Moderate to good tenacity and pleasant, natural-herbaceous undertone.

This ester, although not very commonly offered, finds some use in perfumery as a modifier for the lower homologues of the same series, and for the related Benzyl esters, mainly in fruity-floral complexes such as Jasmin, Gardenia, exotic florals, etc.

It is also used in flavor compositions, particularly in imitation Apricot and Apple. Furthermore in various berry compositions and fruit complexes.

The concentration used is about 5 to 20 ppm in the finished product.

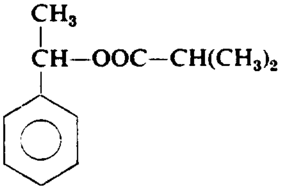
G.R.A.S. F.E.M.A. No.2686.

Prod.: from Methyl phenyl carbinol and *n*-Butyric acid by azeotropic esterification.

34-162; 86-98; 103-292;

## 2180: METHYL PHENYL CARBINYL-iso-BUTYRATE

*alpha*-Methyl benzyl-*iso*-butyrate.
Phenyl methyl carbinyl-*iso*-butyrate.
"Styrallyl-*iso*-butyrate".



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

More ethereal-floral and less fruity than the *n*-butyrate (see preceding monograph). Jasmin-like and warm-herbaceous undertones and moderate tenacity.

This ester, rarely offered commercially, finds a little use in various heavy floral perfume compositions, including Jasmin.

Perfumers seem to have different opinions about Butyrates and *iso*-Butyrates. Some perfumers will claim that, in general, the *n*-Butyrates have more natural odors, while the *iso*-Butyrates are "artificial" in character. Comments about the physical and chemical stability seem to speak in favor of the *iso*-Butyrates in general.

This ester finds limited use in flavor compositions, almost exclusively in fruit complexes. The concentration is normally as low as 2 to 10 ppm in the finished product.

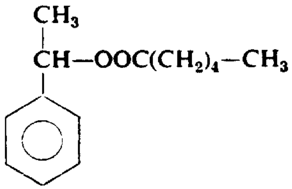
G.R.A.S. F.E.M.A. No.2687.

Prod.: from Methyl phenyl carbinol and *iso*-Butyric acid by azeotropic type esterification.

34-162; 103-292;

## 2181: METHYL PHENYL CARBINYL CAPROATE

*alpha*-Methyl benzyl-*n*-hexanoate.
*alpha*-Methyl benzyl caproate.
Phenyl methyl carbinyl hexoate.
"Styrallyl caproate".



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mild, fruity and sweet odor of good tenacity. The fruity notes have a certain resemblance to those of Linalyl hexanoate, not only in their peculiar dry fruitiness, but also in their Bois de Rose-like sweetness.

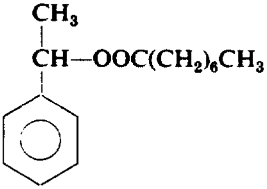
This ester, very rarely offered commercially, is occasionally used in perfume compositions as a mild and sweet background note in floral and floral-woody compositions, often in combination with Ionones or Methylionones. It gives interesting effects in Lavender and it can be used with advantage to extend Clary Sage effects in sweet-herbaceous fragrance types.

Prod.: from Methyl phenyl carbinol and Caproic acid (Hexanoic acid) by esterification under azeotropic conditions.

34-162; 86-98; 103-292;

## 2182: METHYL PHENYL CARBINYL CAPRYLATE

*alpha*-Methyl benzyl octanoate.
Methyl phenyl carbinyl octoate.
"Styrallyl octylate".



$C_{16}H_{24}O_2$ = 248.37

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet, heavy and oily-floral, at times almost fatty odor of moderate to good tenacity.

The odor has some resemblance to that of Geranyl caproate or Geranyl caprylate.

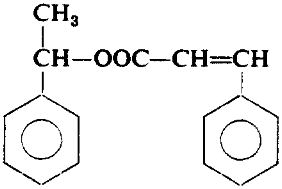
This rare ester finds limited use in perfume compositions, e. g. in Tuberose bases, Lily, Narcissus or Gardenia. It lends effect in those florals similar to what *para*-Cresyl octoate does for a Jasmin: an oily-herbaceous, lasting background note.

Prod.: by direct esterification of Methyl phenyl carbinol with Octanoic acid (Caprylic acid) under azeotropic conditions.

34-162; 86-98; 103-292;

## 2183: METHYL PHENYL CARBINYL CINNAMATE

*alpha*-Methyl benzyl phenylacrylate.



$C_{17}H_{16}O_2$ = 252.32

White crystalline mass.

Insoluble in water, soluble in alcohol (poorly in cold, better in hot alcohol), soluble in most perfume oils.

Practically odorless when pure and freshly prepared. When incorporated in a composition, it may lend balsamic-floral effects to the fragrance, and supply good fixation.

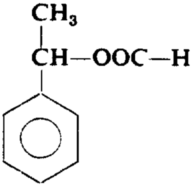
This material finds very limited use in perfumery. It has been suggested as a fixative for Gardenia, and it does have a very attractive effect upon certain types of Gardenia base, particularly those which are not overcharged with Benzylacetate and Methylphenylcarbinyl acetate.

Prod.: by azeotropic type esterification of Methyl phenyl carbinol with Cinnamic acid.

4-130;

## 2184: METHYL PHENYL CARBINYL FORMATE

*alpha*-Methyl benzyl formate.
"Styrallyl formate".
Phenyl methyl carbinyl formate.



$C_9H_{10}O_2$ = 150.18

Colorless mobile liquid.

Slightly soluble in water, soluble in alcohol and oils.

Powerful and dry, green-floral, balsamic-woody odor of Mimosa-Gardenia type. Moderate to poor tenacity.

This ester finds limited use in perfume compositions. Its effect is distinctly different from that of the higher esters in that it is more floral, practically non-fruity. The green notes are dry, not sweet, and they are accompanied by a balsamic undertone.

It finds some use in Hyacinth, Lilac, Apple-blossom, Mimosa and variations of Gardenia, but its main use is in flavor compositions.

Its peculiar dry notes are repeated in the taste, but there is an indirect fruity effect, too.

Smaller amounts are used in various fruit complexes and in berry complexes, Gooseberry, Rhubarb and Blackcurrant, etc.

Concentrations vary from 2 to 20 ppm in the finished product.

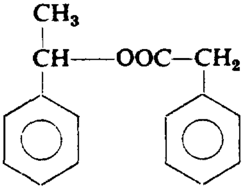
G.R.A.S. F.E.M.A. No.2688.

Prod.: by direct esterification of Methyl phenyl carbinol with Formic acid (usually in presence of Acetic anhydride).

34-162; 86-98; 103-292;

## 2185: METHYL PHENYL CARBINYL PHENYLACETATE

*alpha*-Methyl benzyl phenylacetate.
Methyl phenyl carbinyl-*alpha*-toluate.
"Styrallyl phenylacetate".



$C_{16}H_{16}O_2 = 240.30$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Practically odorless when pure. Most commercial products carry a perceptible "phenylacetic" type odor, while a few show that an excess of Methyl phenyl carbinol has been used in the reaction in order to prevent the appearance of dominating Phenylacetic acid notes. The tenacity is excellent, and the overall effect is best studied when the material is incorporated at the rate of 3-5-8% in a composition. Soft, green-woody-rosy notes may be introduced, while honeylike effects are achieved in combination with lower phenylacetates.

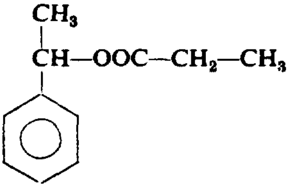
This ester finds limited use in perfume compositions, mainly as a fixative and modifier in heavy or woody florals, in Oriental fragrances etc. It provides generally a "mild Honeysuckle" effect in such fragrances.

Prod.: by esterification of Methyl phenyl carbinol with Phenylacetic acid under azeotropic conditions.

4-130; 103-292;

## 2186: METHYL PHENYL CARBINYL PROPIONATE

"Styrallyl propionate".
*alpha*-Methyl benzyl propanoate.
Phenyl methyl carbinyl propionate.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-floral, sweet and green odor, more refined (less harsh) than the Acetate, more typical of Gardenia and Jasmin, with some resemblance to the green topnotes of Tuberose. In the opinion of many perfumers, this ester is by far superior to the Acetate with respect to attractive, sweet, soft, yet distinctly green-fruity notes. However, a very highly purified Acetate can be virtually free from harsh notes, too.

The title ester is used widely in perfume compositions, as a modifier for or a companion to – the Acetate. It may appear more versatile in that it is not restricted to Gardenia, and it is different from the almost vulgar effect derived from the Acetate, ever since that material was first used in a successful perfume.

Much of the effect of these two esters depend upon the skill and delicate hand using them in a composition, the experience in determining just how much can be used in order to achieve a desirable and attractive effect after proper ageing of the fragrance composition.

This ester works very well with Dimethylbenzyl carbinyl acetate, and related materials with Oakmoss, Clary Sage, Bergamot, Linalool, Lavender, Jasmin, Galbanum, etc.

It is also used frequently in flavor compositions, e. g. in the difficult Gooseberry and other berry imitations, fruit complexes, etc.

The concentration used is normally about 5 to 15 ppm in the finished product.

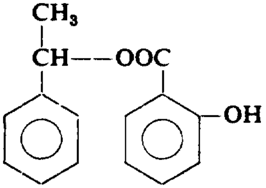
G.R.A.S. F.E.M.A. No.2689.

Prod.: by direct esterification of Methyl phenyl carbinol with Propionic acid, using azeotropic conditions.

4-130; 34-162; 61-71; 86-98; 103-292;

## 2187: METHYL PHENYL CARBINYL SALICYLATE

"Styrallyl salicylate".
*alpha*-Methyl benzyl-*ortho*-hydroxybenzoate.
Phenyl methyl carbinyl salicylate.



$C_{15}H_{14}O_3 = 242.28$

Colorless or white crystals. M.P. 50° C.

Almost insoluble in water, soluble in alcohol and oils.

Practically odorless when pure, very faint, sweet odor of great tenacity. By some observers classified as "musky".

This ester finds limited use in perfume compositions as a fixative and blender in mild floral fragrance types, balsamic or Oriental bases, Lilac, Sweet Pea, Tuberose, Rose, Hyacinth, and in certain sweet-herbaceous, meadow-like fragrance types. It introduces a pleasant and lasting, delicately sweet undertone, supports herbaceous as well as floral notes, and gives a certain warmth to the fragrance, sometimes appearing "powdery", a classification very often wanted.

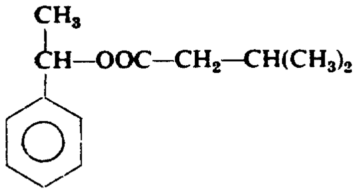
It is used to a minor degree in flavor compositions, in imitation Pineapple, Apricot, Peach, and Honey, normally in traces or little more than traces.

Prod.: by azeotropic type esterification of Methyl phenyl carbinol with Salicylic acid.

34-789; 103-292;

## 2188: METHYL PHENYL CARBINYL-iso-VALERATE

"Styrallyl-*iso*-valerianate".
*alpha*-Methyl benzyl-*iso*-pentanoate.
Phenyl methyl carbinyl-*iso*-valerate.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Herbal-fruity, floral odor of Honeysuckle-Jasmin type. Moderate tenacity.

This ester has not achieved much popularity. It lacks the interesting green notes, usually associated with lower alifatic esters of Methyl phenyl carbinol, and the floral notes of the subject ester are not very characteristic of any natural fragrance.

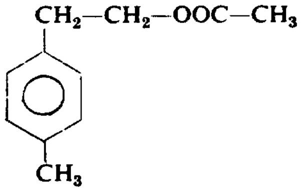
As a modifier in Narcissus, Lily, Jasmin varieties, etc. it can find some application, but most perfume laboratories do not even have the material at their disposal, and probably do not miss this ester.

Prod.: by azeotropic type esterification of Methyl phenyl carbinol with *iso*-Valeric acid.

4-130; 103-292;

## 2189: para-METHYL PHENYLETHYL ACETATE

*2-para* Tolyl ethyl acetate.
*beta-para*-Tolyl ethyl acetate.
"Fliedenol acetate".
"Syringa alcohol, Acetate".
(An isomer of Methyl phenyl carbinyl propionate).



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid. Sp.Gr. 1.03.
B.P. 233° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and relatively pleasant, floral odor of moderate tenacity. The floral notes resemble Lilac and Mimosa.

This ester, usually marketed under trade names, finds use in perfume compositions, mainly soap perfumes of the floral or floral-Oriental type. It is inexpensive and stable, non-discoloring, and sufficiently mild that large proportions can be used without the appearance of dominating or unpleasant notes. It seems to improve the Lilac effect of Terpineol and it can link it pleasantly to Dimethyl benzyl carbinol or related materials. It is not confined to Lilac compositions, and Hydroxycitronellal or Cyclamenaldehyde, or even the "rose alcohols" may blend with this ester into quite a wide range of other floral fragrance types.

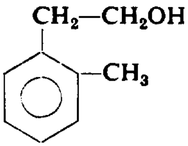
Prod.: from *para*-Tolyl Magnesium bromide plus Ethylene chlorhydrin followed by Acetylation of the alcohol.

86-129;

## 2190: ortho-METHYL PHENYLETHYL ALCOHOL

*ortho-2*-Tolyl ethan-*1*-ol.

This material also forms part of commercial products called *aryl*-Methyl phenylethyl alcohol.



$C_9H_{12}O = 136.20$

Colorless oily liquid. B.P. 219° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and mild, floral odor of Lilac-Rose type. Moderate to poor tenacity. Samples of different origin have shown considerable variation in odor characteristics. This may be due to the fact that commercial products almost inevitably contain *meta*-isomer, probably also *para*-isomer.

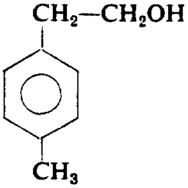
The subject alcohol finds some use in perfume compositions as a base for inexpensive Lilac, Rose, Honeysuckle and other floral fragrance types, and in Fougères, Chypres, etc. It gives modifying notes to a Hyacinth and blends very well with all the Cinnamic derivatives.

Prod.: from *ortho*-Tolyl magnesium bromide plus Ethylene chlorhydrin.

68-500;

## 2191: para-METHYL PHENYLETHYL ALCOHOL

*para-2*-Tolyl ethan-*1*-ol.
"Syringa alcohol".
"Fliedenol".
"Tolyl ethylalcohol".



$C_9H_{12}O = 136.20$

Colorless liquid. Sp.Gr. 1.01. B.P. 222° C.

Almost insoluble in water, soluble in alcohol and oils.

Refined and delicately floral, balsamic-green and rosy odor. Undertones of green-musty, sweet-cinnamic character. Moderate tenacity.

This alcohol, marketed by several different large chemical manufacturing companies over the past many decades with very little success, is still available from various perfume chemical houses.

It is often sold under a trade name, sometimes "bouquettet" with a trace amount of a powerful floralizer.

It finds use in perfume compositions as a base for mild floral fragrance types, Lilac, Rose, Hyacinth, Acacia, Mimosa, etc. and as a blender in many Oriental or non-floral types. Of the three isomers, it is undoubtedly the most popular. However, the commercial product often contains some *meta*-isomer.

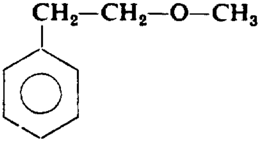
The Acetate of subject alcohol is also a well known perfume chemical.

Prod.: from *para*-Tolyl magnesium bromide plus Ethylene chlorhydrin.

4-111; 4-135; 68-500;

## 2192: METHYL PHENYLETHYL ETHER

Phenylethyl methyl ether.
Methyl phenethyl ether.



$C_9H_{12}O = 136.20$

Colorless mobile oil. B.P. 187° C.

Almost insoluble in water, soluble in alcohol and oils.

Very powerful, diffusive and penetrating odor, warm-floral, but when undiluted rather "gassy"-pungent. In dilution Jasmin-Tuberose-like, floral, sweet. In extreme dilution the odor is even slightly rosy.

The title ether, a rare material in Nature except in Pandanus oil of which it forms the chief constituent, is available as a synthetic chemical. It finds some use in perfume compositions as a powerful and "lifting" ingredient in Hyacinth, Rose, Jasmin, Lilac, Pikake or other heavy exotic florals. It is, naturally, also used in the preparation of artificial Pandanus oil, also known as "Kewda oil" or "Keora oil".

Its volatility makes it somewhat difficult to apply, unless a very solid and "graduated" fixation is constructed around this item.

Styrax, Linalool, Phenylethylalcohol, Dimethyl benzyl carbinyl acetate etc. are useful intermediate blender-fixatives for this material.

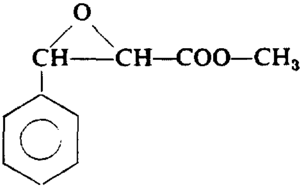
Prod.:

1) from Phenylacetaldehyde dimethylacetal by catalytic reduction.
2) from Phenylethyl alcohol and Methanol by dehydration.

90-675; 104-504;
see also: Ethyl phenylethyl ether.
Ethyl-*ortho*-methoxy benzylether.

## 2193: METHYL PHENYL GLYCIDATE

Methyl-*beta*-phenylglycidate.
Methyl-*alpha-beta*-epoxy phenylpropionate.
Methyl-*alpha-beta*-epoxyhydrocinnamate.



$C_{10}H_{10}O_3 = 178.19$

Colorless oily liquid. Sp.Gr. 1.18.
B.P. 257° C.

Almost insoluble in water, soluble in alcohol and oils.

Mild-fruity, slightly Pineapple-like, sweet odor.

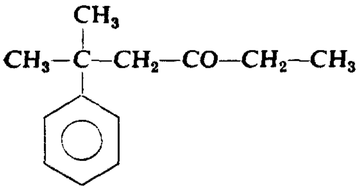
Sweet-fruity, Pear-Pineapple-like taste in dilutions below 20 ppm. Higher concentrations show a slightly bitter taste.

This glycidic ester has been suggested for use in flavor compositions, but is not included in the American G.R.A.S. list. It could find some use as a modifier in Tutti-frutti complexes or in fruity chewing gum flavors, where its fixative value can be utilized.

Prod.: from Benzaldehyde and Methyl monochloroacetate with Sodamide or Sodium methylate as condensing agent.

28-539; (Riechstoffe und Aromen, August 1956, 234).

## 2194: 2-METHYL-2-PHENYL HEXANONE-4



$C_{13}H_{18}O = 190.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Woody-dry, camphoraceous odor of moderate tenacity. In dilution remotely reminiscent of Rose.

Subject ketone has been suggested for use in perfume compositions as a blender and fortifier in Rose and other floral compositions.

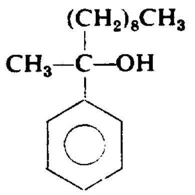
Its camphorceaous character restricts is use to soap perfumes, where power and lift is of paramount importance. For ordinary cosmetic fragrance use, the ketone can be used in discrete amounts, depending upon the fragrance type.

Marketed under trade names, it has not achieved wide distribution, and it is apparently not very successful within the narrow circles of manufacturing users.

Prod.: from *alpha-alpha*-Dimethyl phenylethyl ethylcarbinol by oxidation.

## 2195: METHYL PHENYL NONYL CARBINOL

Nonyl methyl phenylcarbinol.
Methylnonyl phenylcarbinol.
*2*-Phenyl-*2*-hydroxy undecane.
*2*-Phenyl-*2*-undecanol.



$C_{17}H_{28}O = 248.41$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

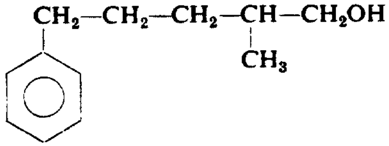
Very mild, herbaceous-woody-oily odor of good tenacity but of rather uninteresting type. The immediate impression is that it lacks character, lacks similarity to anything natural.

This carbinol was probably developed in line with a large number of lower homologues, and the success of certain carbinols encouraged a wider search. The starting material for this carbinol may have tempted the inventors to expect interesting results, but this carbinol never seem to interest the perfumers. It is not a particularly low-cost product, and it has very little odor value. Therefore, it may be reasonable to say that the material is about to become obsolete in perfumery.

Prod.: from Methyl nonyl ketone and Phenylmagnesium bromide in Ethylether solution (Grignard reaction).

## 2196: 2-METHYL-5-PHENYLPENTANOL-1

*beta*-Methyl-*beta*-phenylpropyl ethanol.



$C_{12}H_{18}O = 178.28$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Woody-floral-rosy odor of considerable tenacity.

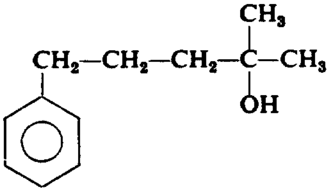
This alcohol and a number of its isomers (see four monographs before and after this) have been suggested for use in Rose bases and new variations of Rose fragrance.

It has not achieved quite the same amount of fame and popularity as its relative, *2*-Methyl-*5*-phenylpentanol-*2*, but it seems that all of these chemicals have lost out in competition with the numerous new fragrance chemicals of literally all odor types, now available at very low cost. Several of these Methylphenylpentanols are still used as part of well-known specialties, or they constitute the entire material in certain fragrance chemicals, marketed undre trade name.

4-248;
See also: *2*-Methyl-*2*-phenylpentanol-*4*.
*2*-Methyl-*5*-phenylpentanol-*2*.
*2*-Methyl-*5*-phenylpentanol-*3*.
*3*-Methyl-*5*-phenylpentanol-*1*.

## **2197:** 2-**METHYL**-5-**PHENYLPENTANOL**-2

Dimethyl phenylpropyl carbinol.
Dimethyl hydrocinnamyl carbinol.
This material is mainly sold under trade names.



$C_{12}H_{18}O = 178.28$

Colorless, slightly oily liquid.

Very poorly soluble in water, soluble in alcohol and oils.

Sweet woody-floral, mildly green odor of good tenacity.

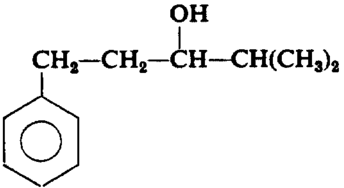
This "carbinol" has been suggested for use in variations of Rose, bases, etc. for its warm-green-floral effect. Several specialties on the market are based solely or mainly upon this chemical.

It blends excellently with Rose materials, Muguet and Lily, Cinnamic alcohol and derivatives, Butylcyclohexanyl acetate, etc.

4-248;
See also: *2*-Methyl-*2*-phenylpentanol-*4*.
*2*-Methyl-*5*-phenylpentanol-*1*.
*2*-Methyl-*5*-phenylpentanol-*3*.
*3*-Methyl-*5*-phenylpentanol-*1*.
and: *iso* Butylbenzylcarbinol.

## **2198:** 2-**METHYL**-5-**PHENYLPENTANOL**-3

*iso*-Propyl phenethylcarbinol.



$C_{12}H_{18}O = 178.28$

Colorless viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Green-woody and slightly floral odor of moderate tenacity.

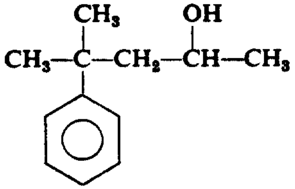
Although closely related to several successful and popular carbinols, this material has not achieved much popularity. It seems to lack natural notes, and its field of application becomes very limited.

Prod.: from Phenylpropionic aldehyde plus *iso*-Propyl magnesium iodide.

4-248;
see also the four isomers of title material before and after this monograph.

## **2199:** 2-**METHYL**-2-**PHENYLPENTANOL**-4

*2*-Hydroxy-*4,4'*-dimethyl-*4*-phenylbutane.
*alpha-alpha*-Dimethyl phenethyl methyl carbinol.



$C_{12}H_{18}O = 178.28$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Woody-peppery, warm and moderately tenacious odor. In combination with floral materials it has the ability to enhance the floral notes, particularly Rose.

This alcohol has been suggested for use in perfumery as a modifier and blender in floral and floral-woody or Oriental type fragrances. It can be used in quite large proportions but this has only interest when the material is available at a reasonable and competitive cost.

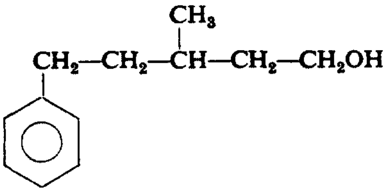
Its odor type is not a particularly desirable one, and its power is not really outstanding. There is reason to assume that this material is on its way to oblivion as a fragrance chemical.

Prod.: (several methods, e. g.): from Phenylmagnesium bromide plus Methyl-*iso*-butylketone to produce the ketone from which the title material is obtained by hydrogenation.

4-109;
see also: 86-62: *2*-Hydroxy-*3*-methyl-*6*-cyclohexyl hexane, and *2*-Hydroxy-*4,4'*-dimethyl-*4*-cyclohexyl butane.
Four isomers of title material are mentioned before and after this monograph.

## 2200: 3-METHYL-5-PHENYLPENTANOL-1

*3*-Methyl-*5*-phenyl-*n*-amylalcohol.
*5*-Phenyl-*active*-hexylalcohol.



$C_{12}H_{18}O = 178.28$

Colorless, slightly viscous liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Green-herbaceous, semi-dry odor with woody undertones, in dilution also floral and with fair to good tenacity.

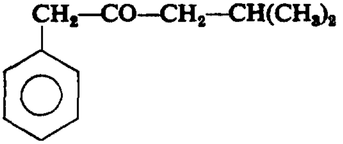
This material is not more interesting than any of its isomers, and there is reason to believe that it will slowly disappear from the perfume laboratory shelves within the next decade or so. Many new materials have power, character, good availability and low cost to tempt the perfumer – virtues that count heavy in the competition among the flood of new aroma chemicals offered every year.

Like its isomers (see previous four monographs) this material has also been offered under various trade names and as a component of perfume bases, but it is no longer of importance.

Prod.: by Grignard reaction with Ethylene oxide and Phenyl-*iso*-propyl magnesium bromide.

## 2201: 4-METHYL-1-PHENYL-2-PENTANONE

*iso*-Butyl benzylketone.
Benzyl-*iso*-butylketone.



$C_{12}H_{16}O = 176.26$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Sweet, but slightly woody-spicy, caramellic-fruity odor of good tenacity.

In concentrations lower than 10 ppm, the taste is sweet, but somewhat tart, fruity-spicy. More fruity at lower concentration, more woody-spicy at higher concentration.

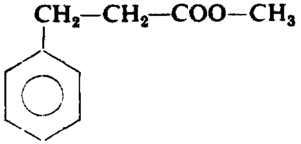
The title ketone is used in flavor compositions, mainly in various berry complexes and in fruit flavors where tenacity is required. The concentration is usually very low because the material has a less pleasant taste at higher levels; 0.05 to 5 ppm in the finished product is common.

G.R.A.S. F.E.M.A. No.2740.

Prod.: by hydrogenation of *iso*-Butyl benzylcarbinol (see that monograph).

## 2202: METHYL PHENYL PROPIONATE

Methyl hydrocinnamate.
Methyl dihydrocinnamate.
Methyl-*3*-phenylpropionate.
Methyl-"*beta*"-phenylpropionate.



$C_{10}H_{12}O_2 = 164.21$

Colorless mobile oil. Sp.Gr. 1.04.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, fruity-winey, fresh-floral and very sweet odor with balsamic-honey-like undertones. Moderate tenacity.

This ester finds use in perfume compositions as a modifying ingredient in Jasmin, Appleblossom, Rose, Lilac, Peony, Carnation, Oriental and many other fragrance types. Its power limits its use to a normal level of a few percent or less in the perfume oil.

It gives much more lift than Methylcinnamate, but it is not nearly as tenacious. It is more floral and less fruity.

The subject material finds also use in flavor compositions, usually in minute traces only, e. g. in imitation Apple, Apricot, Honey, Peach, Pineapple and in "Rose" flavors. Normal concentration is about 0.5 to 2 ppm in the finished product.

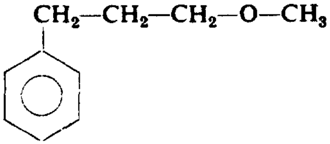
G.R.A.S. F.E.M.A. No.2741.

Prod.: by direct esterification of Methanol with Hydrocinnamic acid, or by controlled hydrogenation of Methylcinnamate.

4-95; 7-279; 34-581; 106-265;

## 2203: METHYL PHENYLPROPYLETHER

*3*-Phenylpropanol, Methylether.
An old name is: *beta*-Phenylpropyl methylether, or: Methyl-*beta*-phenylpropylether. (See NOTE below).
Hydrocinnamyl methylether.
Methyl hydrocinnamylether.



$C_{10}H_{14}O = 150.22$

Colorless liquid. B.P. 207° C. Sp.Gr. 0,99.

Almost insoluble in water, soluble in alcohol and oils.

Pungent floral-balsamic odor of Hyacinth-Orangeblossom-Rose type. Moderate to poor tenacity.

This ether has been suggested for use in perfume compositions as a fortifier for floral, mainly heavy-floral, fragrance, e. g. Hyacinth, certain types of Rose, Lily, Gardenia, etc.

It is rarely offered commercially under its proper name, and there is even the possibility of confusion with the isomer, Methyl hydratropyl ether, see above and below.

Prod.:

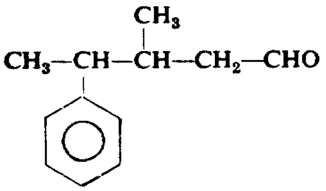
1) by dehydration of a mixture of Methanol and Phenylpropyl alcohol.
2) by reduction of Phenylpropionaldehyde dimethylacetal.
3) from (*gamma*-Chloropropyl)-benzene plus Sodium methoxide.

NOTE: the Methylether of Hydratropyl alcohol (*alpha*-Methyl phenethylalcohol, Methylether) is known, but the author believes that it is not commercially available, and rarely, if ever, manufactured for perfumery purposes.

See also: Methyl phenylethyl ether.
Ethyl phenylethyl ether.
Ethyl-*ortho*-methoxy benzylether.
95-111; 96-92;

## 2204: 3-METHYL-4-PHENYL VALERIC ALDEHYDE

Methyl phenyl pentanal.



$C_{12}H_{16}O = 176.26$

Colorless mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-floral, relatively powerful and herbaceous odor with a tobacco-like, warm undertone.

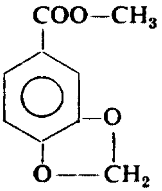
This aldehyde, rarely seen under its proper chemical name, has been suggested for use in perfume compositions, mainly for novel notes in Chypre, Fougères, as a background in Rose or Oriental types, or in Men's "Leather" perfumes.

It blends very well with Oakmoss products, Amylsalicylate, Lavender and Labdanum products, etc. and could find use in sophisticated Pine needle fragrances. Its cost does not allow for everyday use for that purpose.

Prod.: by oxidation of *3*-Methyl-*4*-phenylpentanol. A number of isomers of that alcohol are listed in this work.

## 2205: METHYL PIPERONYLATE

Methyl-*3,4*-methylene dioxybenzoate.



$C_9H_8O_4 = 180.16$

Colorless or white crystals. M.P. 52° C. B.P. 257° C.

Almost insoluble in water, soluble in alcohol and oils.

Very mild, dry-herbaceous, almost powdery odor of good tenacity.

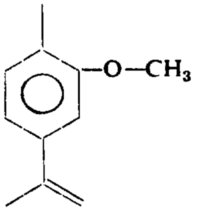
This ester has been suggested for use in perfume compositions, but it does not seem to have achieved popularity of any significance, not even as much (or little) as the Ethyl ester (see that monograph). It could find use in floral-balsamic and powdery fragrance types, particularly in conjunction with Methylionones and Musks, but its odor value is relatively low, and the ester is rarely offered by the conventional manufacturers of perfume chemicals. Therefore, it is too expensive for its effect.

Prod.: from Heliotropine by oxidation with Potassium permanganate to yield Piperonylic acid. Then esterification. The acid can also be obtained directly from Safrole.

47-41; 49-472;

## 2206: METHYL-2-iso-PROPENYL-5-ANISOLE

*2*-Methyl-*5*-*iso*-propenylanisole.
Dehydrocarvacrol methylether.



$C_{11}H_{14}O = 162.23$

Colorless liquid. Sp.Gr. 0.98. B.P. 245° C.

Almost insoluble in water, soluble in alcohol, miscible with oils.

Pungent-dry, medicinal, but refreshing odor of moderate tenacity. There is some similarity to the odor of Thymol, and the odor is pleasantly free from the "tarry" notes found in Carvacrol.

This Phenolether has been suggested for use in perfume compositions, e. g. in modern soaps, where the odor may be expected to imply a bactericidal effect, actually supplied by a separate (and often almost odorless) ingredient in the so-called "deodorant soap bar".

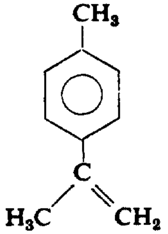
Prod.: the material can be isolated from the essential oil of Chamaecyparis obtusa, known as Hinoki leaf oil, produced in Taiwan (Formosa).

The Phenolether can also be prepared synthetically from Carvacrol by Methylation in weak aqueous alkali, followed by dehydrogenation.

90-464; 104-154;
see also: Helvetica Chim. Act. vol. 48, 1965, page 1057.

## 2207: 1-METHYL-4-iso-PROPENYL BENZENE

"Dehydro-*para*-cymene".



$C_{10}H_{12} = 132.21$

Colorless mobile liquid. B.P. 189° C. Sp.Gr. 0.85.

Insoluble in water, soluble in alcohol, miscible with oils.

Citrusy-lemonlike odor, but rather "gassy"-Styrene-like when undiluted. It bears some resemblance to the odor of Phellandrene.

This hydrocarbon has been suggested for use in perfume compositions, mainly as a component in certain artificial essential oils. In Lemon fragrances for industrial masking purposes it may introduce lift, power and freshness, but its cost is, at the time of writing this monograph (1968), too high to allow for extensive use as a masking agent.

The title material can be hydrogenated to yield a comparatively pure grade of *para*-Cymene.

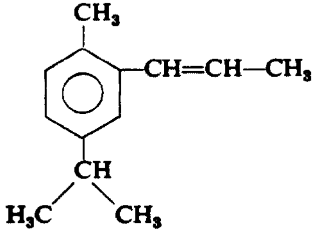
Prod.: the material occurs as a by-product in the rectification of the Formosan oil known as Hinoki leaf oil.

It could also be produced by dehydrogenation of *para*-Cymene.

87-411;

## 2208: 1-METHYL-2-PROPENYL-4-iso-PROPYLBENZENE

"Verdoracine" (Naarden).
*ortho*-Propenyl-*para*-cymene.



$C_{13}H_{18} = 174.29$

Colorless or very pale straw-colored, slightly oily liquid.

Practically insoluble in water, soluble in alcohol, miscible with oils.

Green-earthy odor. The green being almost root-like green with vegetable and dry undertones, reminiscent of Galbanum, Vetiver, Aspargus, Tomato-leaves, etc. and a pleasant, somewhat sweeter, Pine-Savin-like and balsamic terminal note.

This relatively new chemical has been suggested for use in modern fragrances as a modifier to the very popular "green" theme with Oakmoss, Galbanum, Vetiver, Styrallyl-esters, etc. to create fresh and natural-woody nuances, dry-green notes in Men's fragrances, Citrus colognes, "Tabac" notes, etc. It is also an excellent additive in new variations of the "leather" theme.

It is interesting to note that the Asparagus note is also present in the light fractions of freshly produced Vetiver oil. These light fractions have at times been used to imitate the Asparagus odor.

(Naarden, N.V. Chem. Fabr., data sheet 1967).

It is interesting to notice the similarity in odor of this material to that of Allyl pulegone, chemically related to the title hydrocarbon.

## 2209: METHYL PROPIONATE

Methyl propanoate.

$CH_3—OOC—CH_2—CH_3$

$C_4H_8O_2 = 88.11$

Colorless mobile liquid. Sp.Gr. 0.92.
B.P. 80° C.

6.5% soluble in water, miscible with Propylene glycol, alcohol and oils.

Very diffusive, ethereal-Rum-like odor, sweet and fruity of very poor tenacity.

Sweet and fruity taste in concentrations higher than 20 ppm.

This ester finds very little, if any, use in perfumes. Many light and fruity esters are used in trace amounts in perfumes as part of powerful and diffusive topnotes, but this ester is too volatile to yield such desirable effects, even with solid fixation.

It finds extensive use in flavor compositions, mainly in imitation Rum and fruit complexes, "Tutti-frutti", etc. or in traces to introduce the "overripe" or fermented-fruit-effect, sometimes called for. Concentrations vary from 20 to 130 ppm in the finished product.

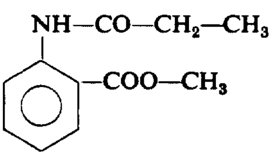
G.R.A.S. F.E.M.A. No.2742.

Prod.: by direct and azeotropic type esterification of Methanol with Propionic acid, or Methanol plus Propionic alhydride.

4-96; 33-620; 26-610; 86-98; 103-80; 104-137; 160-1188; B-II-239;

## 2210: METHYL-N-PROPIONYL ANTHRANILATE

*N*-Propionyl methylanthranilate.



$C_{11}H_{13}NO_3 = 207.23$

Pale straw-colored, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet Petitgrain-like and Grape-like odor of good tenacity.

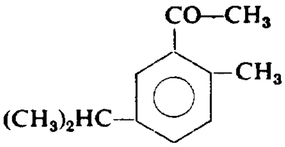
This ester has been suggested for use in perfume compositions as a particularly "Petitgrain-like" Anthranilate. Out of scores of Anthranilic acid esters, only a few have managed to remain in the perfumer's laboratory as standard items. This particular ester has very limited fields of use, and its cost does not place it first on the list of selections, when the perfumer has certain cost limitations (and 98% of all perfumers have, I believe!).

Its mildness and good tenacity, its Neroli-notes free from the undesirable part of the Petitgrain-theme, are among the virtues of this ester. Its acyl-radicle seems to create a hazard of sour notes, building up upon storage of the ester.

Prod.: from Propionyl anthranilic acid (from Anthranilic acid plus Propionic anhydride in Benzene) by Methyl-esterification.

## 2211: METHYL-iso-PROPYL ACETOPHENONE

*5-iso*-Propyl-*2*-methylacetophenone.
Carvacryl methyl ketone.
*2*-Acetyl-*para*-cymene.



$C_{12}H_{16}O = 176.26$

Colorless liquid. Sp.Gr. 0.96. B.P. 240° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, herbaceous-woody, in dilution floral and sweeter odor of good tenacity.

This ketone has been suggested for use in perfume compositions for its powerful effect in Mimosa and Cassie bases, the latter still being quite popular as undertone in many modern perfumes.

It blends well with the Ionones, Anisalcohol and esters, Cinnamic alcohol and esters, Tolu-balsam, Ylang-Ylang, Peru balsam, Benzyl-salicylate and other sweet-balsamic or powdery materials. The Nitromusks offer satisfactory fixation and sweetness to this rather sharp odor, and it will rarely be used at concentrations higher than a few percent.

This material is not often marketed under its chemical name.

Prod.:

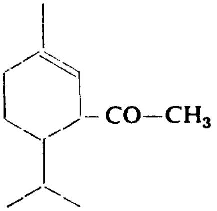
1) from *para*-Cymene with Aluminum chloride and anhydrous Sodium acetate,
   or directly from
2) Toluene with *iso*-Propylchloride and anhydrous Sodium acetate and Aluminum chloride.

See also monograph: Acetocumene – that material contains some *meta*-isomer.

160-782;

## 2212: 5-METHYL-2-iso-PROPYL-1-ACETYL-5-CYCLOHEXENE

*5*-Methyl-*2*-*iso*-propyl-*5*-cyclohexenyl methyl-ketone.
"Cyclocitralone" (Givaudan)
– and other trade names.
The commercial product may be a mixture of *alpha*- and *beta*-isomers.



$C_{12}H_{20}O = 180.29$

Colorless or pale yellowish oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, fruity-woody odor of moderate to good tenacity. There are variations in the odor characteristics, presumably according to purity and isomer ratio. The product is manufactured by several perfume houses under different trade names and in different olfactory quality.

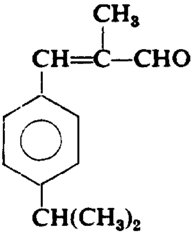
At the time of development, this ketone was quite popular, and it was found to be very versatile in perfumery, blending equally well with floral and fruity and balsamic notes. It was successful in soap perfumes and in various perfume specialties, but has since then been outperformed by newer and more uniform materials.

Prod.: by cyclization of Citralone with sulfuric or phosphoric acid to produce ketones of different isomer-ratio.

31-97;
see also monograph: *5,9*-Dimethyl-*4,8*-decadien-*2*-one (= Citralone).

## 2213: alpha-METHYL-para-iso-PROPYL CINNAMICALDEHYDE

*3*-(*para*-*iso*-Propyl)-*2*-methyl-*2*-propenal.
"Dehydro cyclamenaldehyde".



$C_{13}H_{16}O = 188.27$

Pale yellowish liquid. B.P. 260° C.
Sp.Gr. 0.97.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, but also musty odor of considerable tenacity. The odor has been described as resembling that of dry leaves, and literature uses alternately the words "pleasant" and "unpleasant" odor of dry leaves. This inconsistency is not uncommon in perfumery language, and it shows once more the difficulty in transmitting olfactory observations in a practical and useful manner.

But let it be said, that the "odor of dry leaves" is certainly not desirable in Cyclamenaldehyde, and this occurrence may well happen in the normal process of making Cyclamen aldehyde.

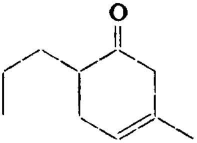
As an isolated perfume material, the title aldehyde could possibly serve as component of certain variations of the spice theme, and it has an interesting effect upon Lavender odor.

Prod.: from Cuminaldehyde plus Propionic aldehyde.

93-151; see also: 156-150;

## 2214: 1-METHYL-4-PROPYL-1-CYCLOHEXENONE-5

An isomer of Piperitone and Carvotanacetone.
Sometimes called:
*3*-Methyl-*6*-propyl-*3*-cyclohexenone.



$C_{10}H_{16}O = 152.24$

Almost colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, in dilution sweet and slightly spicy odor of moderate to poor tenacity. The herbaceous notes are not truly pleasant, except in dilution.

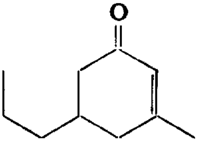
The undiluted material has a rather pungent-chemical odor of nondescript character.

This ketone has been suggested for use in perfume compositions and as a modifier for Carvone. The subject ketone does give interesting effects in Jasmin and Rose (two cases of interesting Carvone-effect), and in proper dilution it forms a pleasant background for Lavender, Lavandin, Geranium, Chypre and Oriental bases, etc. It blends well with Labdanum and Hay notes, e. g. for novel versions of Men's fragrance types.

31-87;

## 2215: 3-METHYL-5-PROPYL-2-CYCLOHEXENONE

"Celery ketone".
*1*-Methyl-*5*-*n*-propyl-*1*-cyclohexen-*3*-one.
An isomer of Piperitone and Carvotanacetone.



$C_{10}H_{16}O = 152.24$

Very pale yellowish or straw-colored, or almost colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, "culinary"-spicy odor of moderate tenacity.

Warm-spicy, woody-haylike taste in concentrations below 20 ppm.

This ketone has found use in flavor compositions for its Celery-like effect and refreshing, powerful aroma, blending very well with Phthalides and other Celery chemicals, and with spices and spice chemicals in general.

It is rarely marketed under its proper chemical name, and does not seem to be very well known, yet it is approved by the authorities in most countries as a food additive (food flavoring and adjuvant).

It could be used in perfumery as an interesting modifier in modern aldehydic Chypres, Fougères, etc., and in connection with Basil and Estragon oils in topnote compositions. It could also find use as a trace ingredient in dentifrice flavors for its contribution to the "biting" mouthfeel, usually supplied by Carvone, and still generally appreciated by the consumers.

The concentration normally used of this ketone is equivalent to 0.3 to 5 ppm in the finished consumer product.

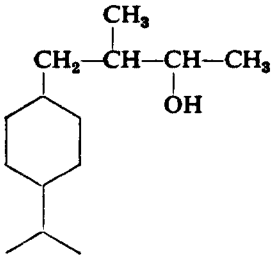
(Approved by the American Federal Register as "Food Flavoring and Adjuvant").

162-669; Recherches: vol. 14, - Dec. 1964, pages 90-92 (Roure-Bertrand Fils & Justin Dupont).

see also: "Bovolide" and
Dihydrocarvone, and
previous monograph.

## 2216: 3-METHYL-4(4'-iso-PROPYLCYCLOHEXYL)-BUTANOL

Sometimes called:
*2*-Oxy-*3*-methyl-*4*(*4'*-*iso*-propylcyclohexyl)-butane-*3*.
*3*-(*para*-Menthanyl)-butan-*2*-ol.



$C_{14}H_{28}O = 212.38$

Almost colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant floral-woody odor of good tenacity. The woody notes are light and fresh, the floral tone is also light, almost green and sweet.

Some observers (and manufacturers) find a Sandalwood odor in this material.

This material has been suggested for use in perfume compositions mainly in floral, floral-woody and Oriental types.

It blends excellently with the Ionones, Lilial or Cyclamenaldehyde, Amylsalicylate, many carbinols, Sandalwood and Patchouli oils, Geranium, etc.

The combination of sweet and woody notes is a comparatively rare one in Aroma chemicals, and any such material that has further assets as a perfume chemical, will be looked upon with the greatest interest. Before 1950, there were but a few such chemicals, but certain of the more recently marketed Sandalwood chemicals have completely taken over the volume-use of artificial Sandalwood notes.

The title material has, in the author's opinion, only little more than academic interest today, but it is included in this work also to illustrate the wide, difference in chemical structure under which we may find Sandalwood odors.

It is a comparatively rare perfume material, and not often seen under its proper chemical name.

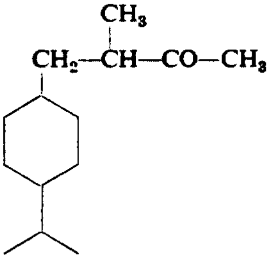
Prod.:

1) by hydrogenation of the corresponding ketone (see next).
2) from Cuminaldehyde by hydrogenation to *para-iso*-Propylbenzaldehyde, which is condensed with Methyl ethyl ketone. The condensation product is hydrogenated to the saturated ketone and further to the secondary alcohol.

4-109;

## 2217: 3-METHYL-4(4'-iso-PROPYLCYCLOHEXYL)-BUTAN-2-ONE

*3-para*-Menthanyl butan-*2*-one.



$C_{14}H_{26}O = 210.36$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

The title material has been suggested for use as a Sandalwood odor, but it has not been marketed yet under its proper chemical name. It was developed long before the very successful Camphenyl derivatives of Sandalwood odor were discovered, and it is quite possible that the subject ketone has lost its importance, which apparently never was very great.

Prod.:

1) from Hexahydro-*para-iso*-propylbenzaldehyde by condensation with Methyl ethyl ketone, followed by hydrogenation.
2) from the corresponding alcohol, see previous monograph.

159-414;

## 2218: METHYL-1-PROPYL DISULFIDE

Methyl-*1-n*-propyl disulfide.

$CH_3—S—S—CH_2—CH_2—CH_3$

$C_4H_{10}S_2 = 122.26$

Pale yellowish mobile liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very powerful, penetrating, sulfuraceous-herbaceous odor of Onion type, but non-lachrymatory and not very tenacious. In extreme dilution sweet and more pleasant "natural" odor.

The title sulfide, which is a major component of natural Onion volatile oil, has been synthesized and finds use in flavor compositions. Its primary use is in Onion flavor, artificial Onion oil (reconstitution of lost natural flavor in processing of Onion), etc.

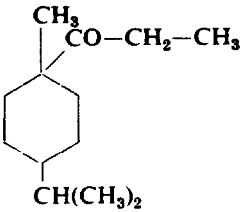
Its flavor is almost identical to its odor, a feature which is quite typical of the powerful natural condiment-components. There is a sweet taste perceptible only if the observer can eliminate the sense of olfaction, but the flavor of Onion is primarily derived from odor. At normal (pleasant) level of concentration there should be no pungency or burning mouthfeel.

Prod.: from Methyl mercaptan plus Propyl mercaptan with Bromine.

60- November -53; 90-825; 158-136;
see also monographs: Dimethyl disulfide (a minor Onion component) – and: Dipropyl disulfide (a major Onion component).

## **2219:** alpha-**METHYL**-para-iso-**PROPYL HEXAHYDRO PHENYLETHYLKETONE**

*1*-(*1*-Methyl-*1*-(*4*-*iso*-propylcyclohexyl))-*1*-propanone.



$C_{13}H_{24}O = 196.34$

Colorless, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Green-woody, floral and relatively sweet odor of good tenacity. The woody notes resemble Amyris and Sandalwood to some degree.

This ketone has been suggested for use in perfume compositions as a blender/modifier for Cyclamenaldehyde and Ionones, e. g. in Mimosa bases, and in delicately woody or woody-musky fragrances types. It performs well in soap, but it is rarely sold under its chemical name and is probably not well known as a fragrance chemical.

It has been offered under a trade name, but is no longer available under that original name.

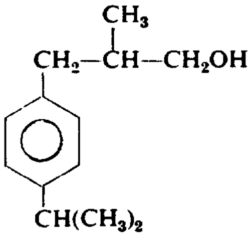
Most likely, the material has failed to live up to expectations, and has been outperformed by newer and more effective chemicals.

Prod.: by hydrogenation of *1*-Methyl-*4*-*iso*-propyl propiophenone.

36-1255; 103-275;

## **2220:** alpha-**METHYL**-para-iso-**PROPYL HYDROCINNAMIC ALCOHOL**

"Cyclamen alcohol".
*para*-*iso*-Propyl-*alpha*-methyl phenylpropylalcohol.
*3*-(*4*-*iso*-Propylphenyl)*2*-methylpropanol.
*2*-Methyl-*3*-cumenylpropanol.



$C_{13}H_{20}O = 192.30$

Colorless, slightly viscous liquid.
Sp.Gr. 0.95.

Very slightly soluble in water, soluble in alcohol and oils.

Mild and sweet, floral odor of delicately green, fresh and lasting character. Does not display the Melon-like greenness of the aldehyde, but is also without the power of that material.

This alcohol, sometimes occurring in the process of making Cyclamen aldehyde, has found some use in perfume compositions, besides of being used as part of a stabilizing composition for Cyclamen aldehyde. The aldehyde has a notoriously poor stability, but modern additives and technique of manufacture has put reasonable limits to the breakdown. The alcohol may form a hemiacetal with the aldehyde, thus creating a "buffer" for the breakdown process. The aldehyde does not suffer significantly from the presence of these derivatives which have acceptable and weaker odors.

Newer processes may avoid the process of making the alcohol, and as a fragrance material, it has never had much popularity. It will most likely become obsolete in the near future.

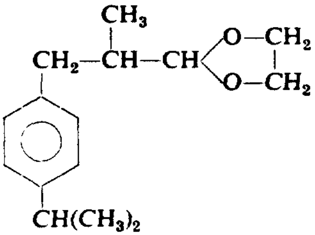
Prod.:

1) as a by-product in the manufacture of Cyclamenaldehyde.
2) from Cumyl ethylcarbinol, or from Cumyl propene.

31-68; 31-70; 34-772; 156-147;
See also 2672;

## 2221: alpha-**METHYL**-para-iso-**PROPYL HYDROCINNAMIC ALDEHYDE ETHYLENEGLYCOL ACETAL**

Cyclamal ethyleneglycol acetal.
Cyclamal cycloacetal.



$C_{15}H_{22}O_2 = 234.34$

Colorless, slightly viscous liquid.
Sp.Gr. 1.00.

Almost insoluble in water, soluble in alcohol and oils.

Very faint, but tenacious, delicately floral and discretely green odor.

This acetal was developed among many at the time when the cyclic acetals were under close observation, since several such acetals had appeared to be of substantial interest to the creative perfumer. Many of these cyclic acetals were almost odorless, a few were of individually interesting and characteristic odor.

The title acetal can not truly be placed in the latter category, and the author is of the impression that it is very rarely used today.

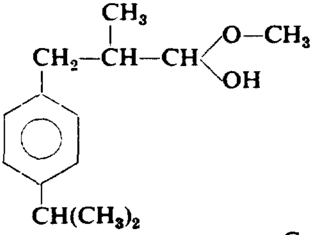
Much more interesting are the acetals of alifatic aldehydes with glycols, often known under their Dioxane- or Dioxalane-structure name.

33-158;

Cyclamen aldehyde is listed as No. 758.

## 2222: alpha-**METHYL**-para-iso-**PROPYL HYDROCINNAMIC ALDEHYDE MONOMETHYLACETAL**

Cyclamal monomethylacetal.



$C_{14}H_{22}O_2 = 222.33$

Colorless oily liquid.

Odor resembling that of Cyclamen aldehyde, but sweeter and milder.

This acetal has found use as a stabilizer for Cyclamen aldehyde.

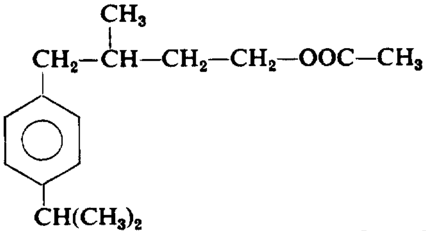
It is estimated that the acetal is about 15% weaker than the aldehyde itself, and the acetal will eventually release its entire charge of aldehyde in active use.

There is very little reason to use the title acetal as an individual fragrance material, and it will probably only remain as a stabilizer as above mentioned. The human nose is notoriously poor when it comes to evaluation of relative strength, and many observers would be unable to tell the difference between Cyclamen aldehyde and a mixture of the aldehyde with the title hemiacetal, even at 50/50 proportion.

31-63; 31-70;

## **2223:** alpha-**METHYL**-para-iso-**PROPYL HYDROCINNAMYL ACETATE**

"Cyclamen acetate":
Cyclamen alcohol, acetate.



$C_{15}H_{22}O_2 = 234.34$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, balsamic-floral odor of very good tenacity, but overall weak.

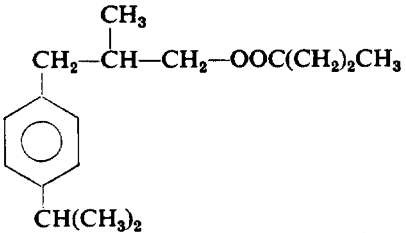
This ester was manufactured many years ago, and the author is of the impression that it is rarely, if ever, manufactured on a commercial scale today.

Apart from being slightly richer and more odorous than the alcohol, it has very little to offer, and nothing really unusual or outstanding. The ester will most conceivably remain in the cabinet with research samples and curiosities, not on the perfumers "active" shelf.

Prod.: by esterification of the alcohol (see monograph).

## **2224:** alpha-**METHYL**-para-iso-**PROPYL HYDROCINNAMYL BUTYRATE**

"Cyclamen butyrate".
Cyclamen alcohol, *n*-butyrate.



$C_{17}H_{26}O_2 = 262.40$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

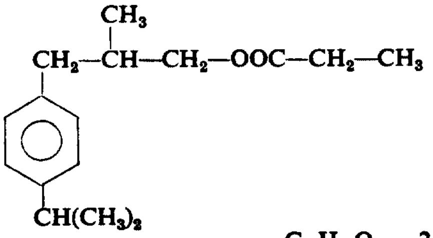
Mild, fruity-floral, sweet and very tenacious odor. Although attractive as an odor, it has very little power and no real character.

This ester was manufactured several decades ago, and offered commercially with very little success. It is rarely offered today, and the author feels that it can be classified as practically obsolete.

Prod.: from Cyclamen alcohol (see earlier monograph) and *n*-Butyric acid by azeotropic type esterification.

## **2225:** alpha-**METHYL**-para-iso-**PROPYL HYDROCINNAMYL PROPIONATE**

"Cyclamen propionate".
Cyclamen alcohol, propionate.



$C_{16}H_{24}O_2 = 248.37$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild, fruity-balsamic, sweet and tenacious odor. Overall of poor strength, almost without character or "type". Only if it were available at a cost well below that of Cyclamal, this ester could probably become of some importance as a modifier/blender in Oriental fragrance types, Hyacinth, Narcissus, Ylang, Lily, etc.

The material was commercially available several decades ago, but has not been offered regularly during the past ten years.

Prod.: by esterification of Cyclamen alcohol (see earlier monograph) with Propionic acid under azeotropic conditions.

## 2226: METHYL PROPYL KETONE

Propyl methyl ketone.
Ethyl acetone.
*2*-Pentanone.

$CH_3—CO—CH_2—CH_2—CH_3$

$C_5H_{10}O = 86.14$

Colorless liquid. Sp.Gr. 0.81. B.P. 102° C.

4% soluble in water, miscible with alcohol, Propylene glycol and oils. The material will dissolve 3.3% water at room temperature.

Powerful and very diffusive, ethereal-fruity odor of "heavy" type (meaning "pungent", but not lasting).

Sweet, ethereal-fruity, Banana-like taste in concentrations below 50 ppm. This ketone finds use in flavor compositions, particularly in the very "radiant" fruit flavors, such as Pineapple and Banana. It is also used in various fruit complexes.

The normal concentration is about 12 to 35 ppm in the finished product.

The title ketone is flammable, and its vapors may form explosive mixtures with air, since the flash point is at room temperature.

G.R.A.S. F.E.M.A. No.2842.

Prod.:

1) by oxidation of *2*-Pentanol.
2) from Methyl ethyl ethylene oxide, by heating.
3) from *n*-Propyl Magnesium bromide plus Acetaldehyde via the alcohol, see 1).
4) from *2*-Pentene and Hydriodic acid via Methyl propyl carbinyl iodide.

(Sample and data, also from Union Carbide Chem. Co.).

26-610; 66-312; 66-516; 100-682; 158-252; 160-1146; B-I-676; 36-1144;

## 2227: METHYL-iso-PROPYL KETONE

*2*-Methyl-*3*-butanone.
*iso*-Propyl methylketone.
Dimethylacetone.

$CH_3—CO—CH(CH_3)_2$

$C_5H_{10}O = 86.14$

Colorless mobile liquid. Sp.Gr. 0.80.
B.P. 95° C.

Slightly soluble in water, miscible with alcohol, Propylene glycol and oils.

Diffusive, ethereal-camphoraceous odor, pleasant in dilution, somewhat pungent-choking when concentrated.

Ethereal-vinous taste, but slightly bitter at concentrations higher than 50 ppm. This is not much higher than the minimum perceptible, and the effective and "pleasant" level is therefore a rather narrow zone.

This ketone, commercially available in volume, has found some use as part of masking odors for industrial purposes. Its low cost and diffusive odor, also partly its very poor tenacity make it a useful masking odor where the objectionable odor is of high volatility (solvents, fuels, acrylic odors, etc.).

For above reasons, there is probably no interest in the title ketone for flavor purposes.

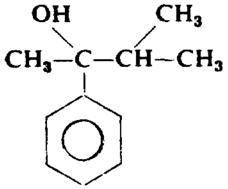
Prod.:

1) by oxidation of Methyl-*iso*-propylcarbinol (*2*-Methyl-*3*-butanol).
2) from *iso*-Propyl magnesium bromide plus Acetaldehyde, followed by reaction as 1).
3) from *2*-Methylbutene plus Hydriodic acid via Methyl-*iso*-propyl carbinyl iodide.

26-610; 31-80; 66-312; 160-884; B-I-682; 61-67; 66-515; 66-516; 66-678;

## 2228: METHYL-iso-PROPYL PHENYLCARBINOL

*3*-Methyl-*2*-phenyl-*2*-butanol.
Methyl-*iso*-propyl benzylalcohol.



$C_{11}H_{16}O = 164.25$

Colorless, slightly viscous liquid, solidifying in the cold. B.P. 230° C.

Almost insoluble in water, soluble in alcohol and oils.

Semi-sweet, green and floral odor of moderate tenacity. More dry, but also richer than *iso*-Propylbenzylalcohol.

This carbinol is not one of the common ones, although it has been available at a very attractive cost. It seems to lack character and versatility in that it does not direct the fragrance towards any particular floral (or green) note, and its power is not nearly comparable to that of e. g. Dimethyl phenylethyl carbinol. The title carbinol has found a little use in Lilac, Hyacinth, Rose and in woody-floral complexes. It also blends well with Lavender in Chypre type fragrances.

Prod.: from Methyl-*iso*-propyl ketone and Phenyl magnesium bromide in a Grignard type reaction.

(See also: 68-501).

## 2229: METHYL-1-PROPYL TRISULFIDE

$CH_3—S—S—S—CH_2—CH_2—CH_3$

$C_4H_{10}S_3 = 154.32$

Pale yellowish, mobile liquid.

Very powerful and penetrating, warm-herbaceous-oily odor of Onion-like character, particularly upon dilution.

Sweet, Onion-like and warm-oily taste in concentrations below 5 ppm.

This material was identified in the volatile oil from fresh Onions only a few years ago during an investigation by which it was also confirmed that Allyl propyl disulfide is not a major ingredient, perhaps not even an important one in the flavor picture of volatile oil from *Onion.*

The title sulfide is considered a relatively important factor for the flavor characteristics of Onion, and it has now been synthesized for use in food flavors, mainly to reconstitute the aroma of Onion lost in the processing of dry foods (soups, etc.).

It was interesting to note that Allyl propyl disulfide is a relatively important, ingredient in *Garlic* volatile oil.

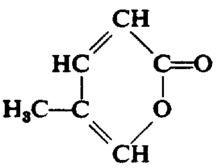
None of the above mentioned type sulfides are lachrymators, and much research has been spent upon identifying the lachrymator of onion. Until writing of this monograph (Sept. 1968) there has been no definite proof, but certain Sulfoxides are under suspicion.

It has also been tentatively evidenced that the lachrymator(s) are not essential to the flavor of Onion. This statement could have been verified by almost any housewife or user of Onion.

158-136; See also: 2938;

## 2230: 5-METHYL-alpha-PYRONE

*5*-Methyl-*2*-pyrone.



$C_6H_6O_2 = 110.11$

White or ivory-colored crystals (in the cold) or pale straw-colored or almost colorless liquid.

The crystals melt at about 19° C.

Slightly soluble in cold water, soluble in hot water and alcohol. Soluble in most oils, poorly in hydrocarbons.

Warm-herbaceous, very sweet and slightly Coumarine-like odor, overall resembling the odor of fresh hay. In dilution more bread-like, but still very sweet and warm.

This ketone has been suggested for use in perfumes and flavors, but its sensitivity to air, alkali and daylight has been a severe drawback to its popularity as an aroma chemical.

Many close relatives of the title material are used in perfumes and even more in flavors.

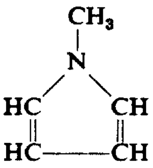
The material could be considered as a prototype of a group of very interesting and promising flavor chemicals, many with good possibilities in perfumery.

See also monographs: Maltol – and: *alpha*-Pyrone.

69-819;

## 2231: 1-METHYL-alpha-PYRROLE

*N*-Methylpyrrole.



$C_5H_7N = 81.12$

Colorless liquid. Sp.Gr. 0.92. B.P. 115° C.

Insoluble in water, miscible with alcohol and oils.

Powerful and penetrating smokey-tarry odor, in extreme dilution sweet, woody-herbaceous, slightly animal. Poor tenacity.

This material has been suggested for use in perfume compositions as trace ingredient in certain floral fragrance types, in artificial flower absolutes, and in minute amounts in animal type bases.

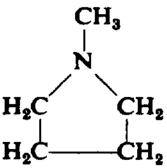
It has also been used in fragrances for industrial purposes ("New-Car-Odors") etc. where a diffusive and distractive odor may be of good effect.

Prod.: by heating of Methyl ammonium mucate.

68-31; 68-41; 160-1204;

## 2232: METHYL PYRROLIDINE

*N*-Methyl pyrrolidine.



$C_5H_{11}N = 85.15$

Almost colorless or very pale straw-colored liquid. B.P. 83° C.

Soluble in water, miscible with alcohol. Soluble in some oils, but not in all.

Warm-herbaceous-animal, in dilution exotic -nauseatingly floral odor of poor tenacity. Trace impurities in commercial grade material often change the odor picture substantially.

This material, much sweeter and "heavier" in odor than Methyl pyrrole, has found limited use in perfume compositions as a trace ingredient in certain types of exotic floral or Oriental-floral-woody fragrance. Its effect is somewhat similar to that of Piperidine (see monograph) which is also used for such purposes.

Prod.: by hydrogenation of *N*-Methylpyrrole over Adams' catalyst.

160-1204;
(see also: 68-62).

## 2233: METHYL QUINOLINES

(summary)

*2*-Methylquinoline = Quinaldine = *alpha*-Methyl-q.
*3*-Methylquinoline = *beta*-Methyl-q. Uninteresting.
*4*-Methylquinoline = Lepidine = *gamma*-Methyl-q.
*5*-Methylquinoline = *ana*-Methyl-q. The highest boiling of all the isomers. Of no interest to perfumery.
*6*-Methylquinoline = *para*-Methyl-q.
*7*-Methylquinoline = "Lilacine" = *meta*-Methyl-q.
*8*-Methylquinoline = *ortho*-Methyl-q.

Of the seven above named isomers, the *3*-Methyl-and the *5*-Methyl- are of no apparent interest to perfumery.

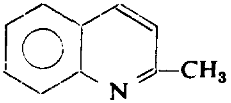
The remaining five would rank in order of perfumery importance *7-6-8-2* – while the *4*-Methylquinoline is the only isomer with any significant interest to the flavor industry.

For physico-chemical data, see: Beilstein, vol. XX, pages 388-401.

See also 1948 = Methylcarbostyril.

## 2234: alpha-METHYL QUINOLINE

*2*-Methyl quinoline.
Quinaldine.
A coal tar product.



$C_{10}H_9N = 143.19$

Colorless liquid or pale amber-colored oily liquid, solidifying in the cold.

M.P. −2° C. B.P. 247° C. Sp.Gr. 1.10.

Slightly soluble in water, soluble in alcohol and oils, poorly in Propylene glycol.

The odor of the commercial product may vary considerably from that of the purified product. There are fishy, "ashtray"-like odors which seem to give way to sweeter, oily herbaceous notes in pure material. The tenacity is good, but the poor grade material has generally unpleasant terminal notes. Light amine-type notes in the initial odor and "extinguished cigar"-odor in the terminal notes are characteristic of commercial grade material.

This Quinoline has found some use in perfume compositions, and even the commercial grade is used for its "tobacco"-like effect which is, indeed, more exhibiting the undesirable notes (ashtray, etc.) than the originally intended (cured tobacco leaves) odor.

However, the title material does not belong to the more popular Quinolines (the *4*- and the *8*-Methylquinolines are among the most frequently used derivatives).

The subject Quinoline may give interesting effects with Civet, Phenylacetic acid, Vetiver, Cedarwood products, etc. and with certain types of Oakmoss.

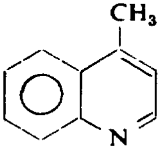
Prod.:

1) by isolation from coal tar quinolines.
2) by Döbner-Miller synthesis from *ortho*-Aminobenzaldehyde and Acetone in Sodium hydroxide solution.

26-612; 68-603; 160-1206; B-XX-388;
(Parfumerie, Cosmetiques, Savons, I, 279, 352).

## 2235: 4-METHYL QUINOLINE

Cincholepidine.
Lepidine.
*gamma*-Methylquinoline.
A coal tar product.



$C_{10}H_9N = 143.19$

Colorless liquid. Acquires a pale straw color or pale amber color upon standing or exposure to daylight. B.P. 263° C. Sp.Gr. 1.09. M.P. 10° C.

Slightly soluble in water, miscible with alcohol and oils.

Powerful, and in high concentration rather repulsive odor of animal-musty character. In extreme dilution the odor becomes pleasant, burnt-oily, herbaceous and floral-sweet of excellent tenacity. It is vitally important that the material is free from homologues and other impurities.

The taste is sweet, floral-oily, slightly burnt in concentrations below 5 ppm.

This Quinoline is used mainly in flavor compositions for imitation Honey, Nut, Butter, Caramel, etc. and in certain fruit complexes. The concentration used is normally about 0.2 to 2 ppm in the finished product.

Prod.: from coal tar.

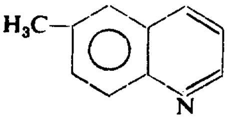
It has also been synthesized from *para*-Aminobenzaldehyde and Acetone.

G.R.A.S. F.E.M.A. No.2744.

26-612; 68-604; 160-1078; B-XX-395; 163-220;

## 2236: meta-METHYL QUINOLINE

7-Methylquinoline.
*meta*-Toluquinoline.
"Lilacine".



$C_{10}H_9N = 143.19$

Pale yellowish oil or almost colorless oil, acquiring a pale amber to brownish color upon exposure to air and daylight. Sp.Gr. 1.07. B.P. 257° C.

Slightly soluble in water, soluble in alcohol and oils.

This is the most floral of the five common isomers of Methylquinoline. In proper dilution it displays a sweet-animal, delicately floral and warm, persistent odor. Although there are perfumers who prefer *para*-Methylquinoline to the title material, there seems to be a general agreement that the *meta*-isomer is more versatile, since it has interesting effect in Lilac, Wistaria, Appleblossom, Hyacinth, Rose (with Civet), Jasmin, Lily, etc., while most of the other isomers are confined to use in Honey, Rose, Civet, Tobacco, etc. or with Oakmoss products in strictly non-floral compositions.

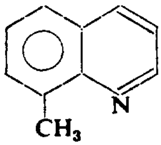
It blends excellently with high-grade Terpineol or Ethyl linalool and with several of the green-floral-earthy carbinols.

Prod.: from *meta*-Toluidine and Glycerol with an Iodine type catalyst in a modified Skraup reaction.

5-307; 26-612; 69-605; 160-1210; 163-48; B-XX-400; 163-44;

## 2237: ortho-METHYL QUINOLINE

*8*-Methylquinoline.
*ortho*-Toluquinoline.
Folianthine.



$C_{10}H_9N = 143.19$

Yellowish or pale amber-colored lily liquid. Sp.Gr. 1.07. B.P. 248° C.
Almost colorless when freshy distilled.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and tenacious, sweet-animal-floral odor with predominantly Civet-Honey-like character. Overall less floral, more Honey-like than the *meta*-isomer.

This material finds some use in perfumery as supporting note in animal-type bases (with Civet, Phenylacetic acid, etc.) and also in minute amounts in variations of Lilac. It has good effects with *iso*-Butylquinoline in modern soap perfumes, but it must be kept at low concentration for such purpose.

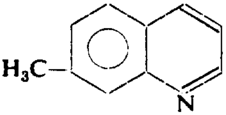
It has also found some use as a fortifier of Ylang and Jasmin-notes in heavy floral and animal-floral bases, and it blends well with Opopanax and Sandalwood for these purposes.

Prod.: from *ortho*-Toluidine by modified Skraup's reaction, using an Iodine catalyst with the Glycerol.

5-307; 26-612; 69-605; 160-1210; 163-358; B-XX-401;

## 2238: para-METHYL QUINOLINE

*6*-Methylquinoline.
*para*-Toluquinoline.
The title name is somewhat misleading, but the author believes that in perfumery literature, the name refers to *6*-Methylquinoline, and not to *4*-Methylquinoline, as one could possibly assume.



$C_{10}H_9N = 143.19$

Pale yellowish or almost colorless liquid. Acquires a brownish color upon standing or exposure to daylight and air.
Sp.Gr. 1.07. B.P. 259° C.

Slightly soluble in water, soluble in alcohol and oils, and in Propylene glycol.

Powerful and penetrating, heavy nauseating odor in high concentration, but sweet, floral-tobacco-like with a discrete Civet-like note when properly diluted (near 1% in odorless or mild, odorous media).

This Quinoline is used in perfume compositions as a fortifier of the heavy and intermediate notes where Tobacco-Civet-Honey-like fragrances are combined to heavy or "exotic" floral notes.

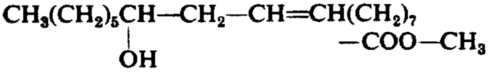
The title material gives interesting variations to the conventional "aldehyde"-theme in the named types of fragrance. It blends well with *iso*-Butylquinoline, Phenylacetic acid and its esters, Jasmin and Gardenia or Tuberose-notes, etc. It is often used in conjunction with Oakmoss products and Ylang-Ylang, or in minute traces as an additive to Phenylethyl-acetate in modern soap perfumes.

Prod.: (many methods) e. g. from *para*-Toluidine and Glycerol by condensation under sulfuric acid conditions with an Iodine type catalyst.

5-306; 26-612; 68-605; 106-266; 160-1210; B-XX-398;

## 2239: METHYL RICINOLEATE

Methyl-*12*-hydroxy-*9*-octadecenoate.



$$CH_3(CH_2)_5\underset{\displaystyle OH}{\underset{|}{CH}}-CH_2-CH{=}CH(CH_2)_7-COO-CH_3$$

$C_{19}H_{36}O_3 = 312.50$

Viscous colorless liquid. B.P. higher than 315° C. (decomposes at atmospheric pressure when heated beyond 300° C.).

Insoluble in water, soluble in alcohol and in most oils.

Virtually odorless when pure, but usually carries a faint, not unpleasant, oily-fatty, mild and bland odor.

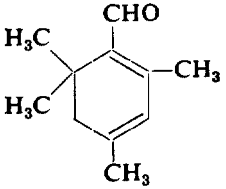
This ester has found limited use in perfumery as a solvent for certain types of Oakmoss extract (mainly for Oakmoss concrete as an emollient or "plasticizer"), and occasionally as part of the "fatty-floral" notes in Jasmin, Gardenia, Tuberose and other herbaceous-oily florals.

Prod.: the acid is obtained from Castor oil by saponification. The Methylester is subsequently obtained by treatment with Methanol and a catalyst or dehydrating agent.

(See also: 66-848).

## 2240: 4-METHYL SAFRANAL

"Homosafranal".
*2,4,6,6*-Tetramethyl cyclohexa-*1:3*-dienal.
*2,4,6,6*-Tetramethyl-*5:6*-dihydrobenzaldehyde.



$C_{11}H_{16}O = 164.25$

Colorless liquid. B.P. approximately 272° C.

Insoluble in water, soluble in alcohol and oils.

Powerful and penetrating, green-herbaceous odor, sometimes described as "ozone-like", or "metallic". In spite of its diffusive power, it is quite tenacious and, when properly diluted, pleasantly fresh, moderately green-condiment-like.

This aldehyde, closely related to the more popular Safranal, is used much the same way, for "space"-odors (room sprays, etc.), and for masking of offensive odors, including household odors. It blends very well with the alifatic aldehydes in Pine fragrances, or with the aldehydes in Citrus oils. It forms novel odors with the green chemicals such as Hexenols, etc. and it gives further lift to woody or woody-camphoraceous notes from Cyclohexanol-derivatives, Ionones, etc.

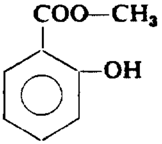
The term "ozone-like" is used quite frequently by perfumers, but it remains poorly defined. There are still unopposed claims that Ozone, as such, is odorless, while secondary products from this highly reactive oxidizing agent may supply various types of odor. The odor appearing when electric energy is discharged in the shape of sparks, may well be "contaminated" with combustion products from ignited dust particles, etc. or other organic and inorganic matter. It is therefore difficult to use the term "ozone-like" odor without further specification.

Prod.: by dehydration of *beta*-Methyl cyclocitral.

51-114; 67-189;

# 2241: METHYL SALICYLATE

Methyl-*ortho*-hydroxybenzoate.
"Synthetic Wintergreen oil".
"Synthetic Sweet Birch oil".
"Synthetic Teaberry oil".



$C_8H_8O_3 = 152.14$

Colorless oily liquid. Solidifies in the cold, melts again at −9° C. Sp.Gr. 1.18.
B.P. 223° C.

0.07% soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Warm, sweet, rooty-fruity odor of moderate to poor tenacity.

Pungent-sweet, fruity-rooty odor with burning sensation at high concentration. As a result of the subconscious reaction in people who are regular users of candy, flavored with Methylsalicylate, or dentifrice etc., the comment "minty" is often used for description of the flavor or odor of this ester. The most reliable judges for *odor* description are those who are not users of the item as a *flavor*.

In fact, the title material is a typical example of an aroma-chemical with widely different end-uses, and, consequently, having widely different descriptions of its odor and flavor attached to it.

Since the material was used mainly as an industrial masking odor in Europe (perfuming of gummed paperstrips, labels, glue, etc.), while it was originally (in the shape of natural Wintergreen oil) an American flavor, an American-Indian Tea, a folksmedicine, and later, the most popular chemical flavoring agent for candy and soft drinks through many decades – the ester will obviously have very different odor/flavor descriptions in different countries. In this respect it resembles Sassafras/Safrole very much.

Methyl salicylate is used in perfume compositions as a minor ingredient in many types of heavy "exotic" floral fragrance, e. g. Tuberose, Cassie, etc. and in artificial Ylang-Ylang. Traces may support other types of floral note, and it may form the sweet undertone in Fougère. Logically, the only aromatic chemical of perfumery (fragrance) interest in fern rhizomes (Fougères) would be Methyl salicylate, since the common fern does not contain any other volatile matter of importance. Amyl salicylate is used more widely because it supplies enormous tenacity, power and sweetness without the distinctly "candy-like" (in the U.S.A.) odor of the Methylester.

The title ester is widely used in flavor compositions, and often forms the chief ingredient, if not the only flavor ingredient, in certain types of consumer product.

It finds use as a minor component in many imitation fruit flavors, e. g. Strawberry, Grape, Blackcurrant, etc., and in Walnut, Vanilla, Spice blends, etc. It supplies a peculiar "green" note in fruit flavors.

It forms a major ingredient in root beer flavor (an American specialty) a variety of which is called "birch beer", and in Wintergreen flavor, "Sarsaparilla" flavor, combination mint flavor, etc.

The average concentration is 25 to 1000 ppm in most finished products, but it may be in excess of 8000 ppm in toothpaste (equivalent to a concentration of approximately 0.8% in the toothpaste, often constituting the entire flavor).

At a meeting in the American Essential Oil Association on Oct. 23, 1962, it was recommended to use the following maximal dosages: from 70 to 150 ppm in candy and carbonated beverages or other digestible foodstuffs.

About 3000 ppm in chewing gum or toothpaste.

Needless to add that these figures are "recommended" and that actual use figures are often much higher.

Pharmacological reports indicate that lethal dosage of Methyl salicylate is about 10 grams for a child and about 30 grams for an adult – within a 24-hour period. It is not unheard of, that children "eat" toothpaste, and it will take 1200 grams or about 8-10 tubes of toothpaste flavored with 0.8% Methylsalicylate to supply the lethal dose of the ester. It would take more than 10 liters of soft drink to arrive at a similar hazardous amount, or about 3 kilos of chewing gum. The alarmingly high number of poison-cases of Methylsalicylate in children per year in the U.S.A. may therefore be attributed to other products, flavored with the ester.

Prod.: by direct esterification of Salicylic acid, using a large surplus of Methanol to reduce the temperature and thus avoid phenolic decomposition of the sensitive acid.

G.R.A.S. F.E.M.A. No.2745.

5-266; 34-788; 26-612; 77-193; 85-87; 90-561; 100-683; 104-659; 106-267; 140-150; 156-325; 160-1220; 163-52; 163-224; 164-325; B-X-70;

## 2242: METHYL STEARATE

Methyl octadecanoate.

$C_{17}H_{35}COO—CH_3$

$C_{19}H_{38}O_2 = 298.51$

White or opaque or colorless crystals.
M.P. 38° C. B.P. higher than 310° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Virtually odorless when pure, but may carry a faint or mild, "refined Castor oil" type of oily odor. Good tenacity.

Practically tasteless, but imparts an oily mouthfeel without being fatty or greasy.

This ester finds a little use in perfume formulations as a blender/modifier or diluent of very little odor value. It may contribute a faint, oily note to flower bases, and it may be useful as an Oakmoss extract solvent, but beyond these and a few other uses, the material is not needed in a perfume laboratory.

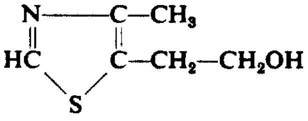
Being a saturated alifatic ester, it is safe against oxidation and rancidity, provided it has been manufactured from a high-grade Stearic acid.

Prod.: by esterification of Stearic acid with Methanol.

26-612; 160-1226; B-II-379;

## 2243: 4-METHYLTHIAZOLYL ETHANOL-5

*5-beta*-Hydroxyethyl-*4*-methylthiazole.
A cleavage product of Vitamin B-1.



$C_6H_9NOS = 143.21$

Pale yellowish liquid, solidifying in the cold.
B.P. 260° C.

Practically insoluble in water, soluble in hot alcohol and oils, poorly soluble in cold alcohol.

Sweet, animal-herbaceous and very tenacious odor.

This rare material has occasionally found use in perfume formulations as a modifier/fixative in Oriental and heavy-floral fragrance types. It blends well with Opopanax and Patchouli, and it forms interesting undertones in Rose. However, it needs support from more powerful odorants since it does not have much character of its own.

Prod.:

1) from Methyl-*alpha*-chloro-*gamma*-hydroxypropylketone and Thioformamide.
2) from Methyl-*alpha*-bromo-*gamma*-acetoxypropylketone with Barium thiocyanate. The resulting *2*-Hydroxythiazole is subsequently converted into the corresponding Thiazole.

69-398;

## 2244: 3-METHYL THIOPROPIONALDEHYDE

*3*-Methylthiopropanal.
Methional.
*beta*-Methiopropional.
Methyl-*beta*-mercaptopropionaldehyde.

$CH_3—S—CH_2—CH_2—CHO$

$C_4H_8OS = 104.17$

Pale yellowish mobile liquid. B.P. 165° C. Sp.Gr. 1.04.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and diffusive Onion-and-meat-like odor, in dilution more pleasant, less Onion-like, reminiscent of "bouillon".

The taste in concentrations of less than 5 ppm is pleasant, warm meat- or soup-like, at higher concentrations with a slight "bite" or pungency.

The title aldehyde, widely distributed in common natural foods, is used in a great number of imitation flavors, mainly cheese, meat and fruit flavors, but also in minute traces in spice blends, concentrated soup (flavors) etc.

The concentration used is so small that it is equivalent to about 0.01 to 2 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2747.

Prod.:

1) (in Nature) by transamination and decarboxylation of various amino acids.
2) by oxidation of the alcohol (see *3*-Methyl thiopropyl alcohol).

140-176; 157-349; 158-82; 158-91; 163-361;

## 2245: 3-METHYL THIOPROPYL ALCOHOL

*3*-Methyl thiol propylalcohol.
*gamma*-Hydroxypropyl methylsulfide.
*gamma*-Methyl mercaptopropylalcohol.
*3*-Methyl thiopropanol.
Methyl-*3*-hydroxypropyl sulfide.
Methionol.

$CH_3—S—CH_2—CH_2—CH_2OH$

$C_4H_{10}OS = 106.19$

Pale yellowish, mobile liquid. B.P. 195° C. Sp.Gr. 1.03.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and sweet soup-or-meat-like odor and flavor. In the undiluted form, the material displays a rather repulsive odor with perceptible notes of sulfuraceous character. Only upon extreme dilution there is a marked improvement to the agreeable and pleasant, food-like note.

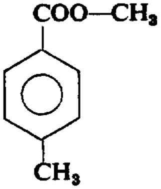
This alcohol has been identified in the volatile portion of Soy sauce, and it was subsequently synthesized for use in food flavors. It is not specifically listed as G.R.A.S. in the American Federal Register or mentioned by the F.E.M.A., but the material is used in other countries and may eventually become a permissible flavor chemical in the U.S.A. The corresponding aldehyde, which has been known for a longer period by the flavor industry, is recognized as a safe flavor chemical (see monograph).

Prod.: from Propylene chlorhydrin and Sodium hydrosulfide.

90-825; 158-91;

## 2246: METHYL-para-TOLUATE

Methyl-*para*-methylbenzoate.
"M-p-T" (Hercules Powder Co.).



$C_8H_{10}O_2 = 150.18$

Crystalline mass or colorless oily liquid. The liquid may remain supercooled for a considerable length of time, although the melting point of the crystals is about 34° C. B.P. 217° C.

Insoluble in water, soluble in alcohol and oils.

Very tenacious, powerful, sweet anisic-floral odor with some resemblance to notes in Ylang-Ylang.

This material, manufactured on a very large scale for purposes other than perfumery (it is a chemical intermediate) has found considerable use in perfume compositions, partly because of its ready availability, partly because of its low cost and good stability.

It offers interesting and pleasant variations in the Methylbenzoate theme in Ylang-Ylang, and it introduces powerful, floral notes in soap and detergent perfumes or, thanks to its low cost, it may be used even in fragrances for masking of industrial odors.

Since the material is manufactured on a very large scale, one must expect that it does not always meet the perfumer's approval on odor. The perfume industry absorbs but a small fraction of the production, and can therefore not be favored with special attention to "odor standards" unless an exceptional premium price is paid. However, it should be added in all fairness to one large manufacturer, that the odor quality is exceptionally high – in view of the above mentioned situation.

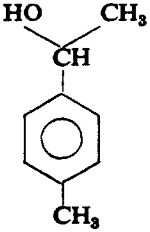
Occasionally, one finds a drum exhibiting a peculiar "fishy" amine-type off-odor, which however will air out after a day or two of open-air agitation at 40° C. The off-odor seems to reveal the method of production (see below).

Prod.:
1) from *para*-Toluidine via the Nitrile to the acid and finally to the Methylester.
2) from *para*-Xylene by oxidation to *para*-Toluic acid, which is subsequently esterified with Methanol.

26-612; 68-544; 160-1254; B-IX-484;
(Hercules Powder Co., Wilmington, Delaware, U.S.A.).

## 2247: METHYL-para-TOLYLCARBINOL

*para-alpha*-Dimethylbenzylalcohol.
*para*-Methyl phenyl methyl carbinol.



$C_9H_{12}O = 136.20$

Colorless, slightly oily liquid. B.P. 219° C. Sp.Gr. 0.96.

Slightly soluble in water, soluble in alcohol and oils.

Rather dry-menthol-like, camphoraceous odor with a faintly woody note and moderate tenacity.

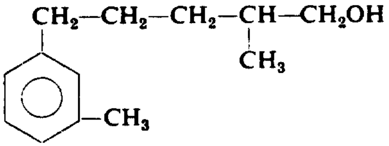
This secondary alcohol has been suggested for use in soap perfumes as a modifier/blender in Rose and Wood type fragrances. It blends well with the "rose" alcohols, but it does steal some sweetness from them. It can give interesting variations in the Ionone theme, and support the woody notes in Lavender-Fougère compositions. But it lacks that touch of naturalness, that trace of a note which recalls just something natural – the effect that may make the difference between liking and disliking the chemical on first impression.

Prod.:
1) from Acetaldehyde and *para*-Tolyl magnesium bromide.
2) by reduction of *para*-Methylacetophenone with Sodium alcoholate.

88-391; 89-458;

## 2248: 2-METHYL-5-meta-TOLYL PENTANOL

*5*-(*3*-Methylphenyl)-*2*-methylamylalcohol.



$C_{13}H_{20}O$ = 192.30

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

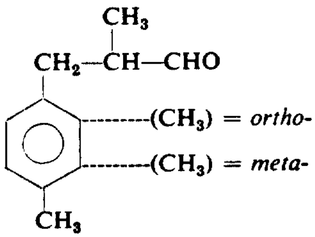
Sweet and green-floral odor with a mildly woody note and good tenacity. Overall rosy character.

This carbinol, very rarely offered under its proper chemical name, has been suggested for use in perfume compositions as a modifier/blender for Rose and woody perfume types, for Oriental fragrances with Sandalwood and Styrax, and in mild florals such as Lily, etc.

Prod.: from *meta*-Tolylpropionic aldehyde by condensation with Propionaldehyde, followed by hydrogenation of the unsaturated *alpha*-Methyltolylpentanal to the title material.

## 2249: 2-METHYL-3-TOLYL PROPIONALDEHYDE

The commercial product consists mainly of *para*-isomer, with some *ortho*-isomer and traces of *meta*-isomer.



*para*-isomer. $C_{11}H_{14}O$ = 162.23

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Intensely sweet, fruity-balsamic odor with variable amounts of Bitter-almond undertones. These are probably results from certain isomers or impurities in the commercial product. A highly purified single isomer is said to have a purely sweet-balsamic and fruity odor.

This aldehyde (complex) is used in flavor compositions as a powerful additive to fruit blends, particularly Raspberry, but also in "tutti-frutti" and similar modern blends for chewing gum and soft candy, or for desserts.

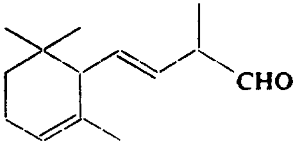
The concentration used is normally mere traces, from 0.05 to 1 ppm in the finished product.

Prod.: from Tolyl aldehyde (*ortho-meta-para*-mixture) by condensation with Propionaldehyde, followed by hydrogenation.

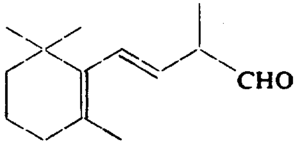
G.R.A.S. F.E.M.A. No.2748.

## 2250: 2-METHYL-4-(2,6,6-TRIMETHYL-1-CYCLOHEXENYL)-3-BUTEN-1-AL

This monograph includes the *alpha*-isomer: *2*-Methyl-*4*-(*2*,*6*,*6*-trimethyl-*2*-cyclohexenyl)-*3*-buten-*1*-al.



*alpha*-isomer.



*beta*-isomer (title material).

$C_{14}H_{22}O = 206.33$

Pale straw-colored, slightly viscous liquid. The color increases during storage, particularly if the material is exposed to daylight and/or air.

Sweet, woody-fruity and very tenacious odor with considerable resemblance to the odor of dried figs (see also monographs: Ionone ethyl glycidate and Ionone methyl glycidate).

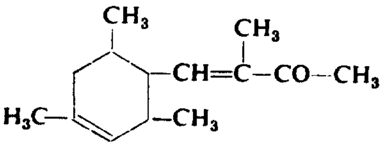
The taste is sweet and fig-or-date-like at concentrations lower than 10 ppm. Higher concentrations seem to produce a "perfumey" and slightly bitter-woody taste.

The title material – and its *alpha*-isomer companion – is used in perfume compositions as a modifier for Ionones or Methylionones in sweet-woody, Oriental or heavy floral-spicy fragrance types, where the excellent tenacity of the title material can be utilized, e. g. in combination with Vetiver products and traces of Undecanolide.

It is interesting to compare this material to: *2*,*2*-Dimethyl-*3*-(*2*,*6*,*6*-trimethyl-*2*-cyclohexen-*1*-yl)-propionitrile (which is described in this work under the above name).

Prod.: from Citral by condensation with Dimethylacetaldehyde. After cyclization a mixture of two isomers result. The isomer ratio can be controlled to a limited degree.

## 2251: 3-METHYL-4-(2,4,6-TRIMETHYL-3-CYCLOHEXENYL)-3-BUTEN-2-ONE



$C_{14}H_{22}O = 206.33$

Colorless or almost colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Delicately woody, tenacious and moderately sweet odor with some resemblance to certain types of Methylionone.

This empirical isomer of Methylionone has found some use in perfume compositions as a novel note and modifier for Methylionones, particularly in the "powdery" type of fragrance, where the Methylionone content is relatively high, and a combination with Musks, Sandalwood and Olibanum is likely.

The lower homologues, some of which are mentioned in this work, have achieved considerable popularity and have been marketed under various trade names for several decades – see:

*4*-(*2*,*4*,*6*-Trimethyl-*3*-cyclohexen-*1*-yl)-*3*-buten-*2*-one,

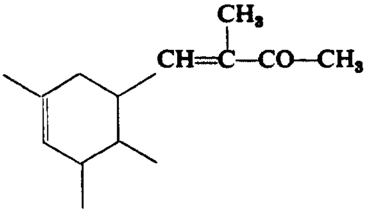
and:

Trimethyl tetrahydrobenzal acetone.

These materials are also isomers of Cyclocitrylidene acetone (Pseudo Ionone).

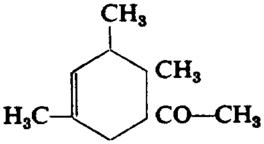
Prod.: (title material): by condensation of *iso*-Cyclocitral and Methyl ethyl ketone.

If the *symmetric-iso*-Cyclocitral is used, the title material will result, but the commercial material usually contains a considerable amount of ketone derived from the *meta-iso*-Cyclocitral:



*3*-Methyl-*4*-(*2,3,5*-trimethyl-*4*-cyclohexenyl)-*3*-buten-*2*-one.

## 2252: METHYL-3,5,6-TRIMETHYL-3-CYCLOHEXENYL KETONE



$C_{11}H_{18}O = 166.27$

Almost colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-camphoraceous, rosy-citrusy odor of moderate tenacity.

This ketone represents one of many results from research following the development of *iso*-Cyclocitral by a Diels-Alder type reaction.

The material has been used in perfume-compositions, particularly in soap and detergent perfumes, but has never gained much popularity. It is rarely offered under its proper chemical name, although it is well known as a chemical, and most houses have or have had some type of the material in their odor library.

It blends well with the "rose alcohols" and with Citronellol in particular, but it is often "lifted" with Benzylacetate, Phenylethylalcohol, *iso*-Butylphenylacetate, etc.

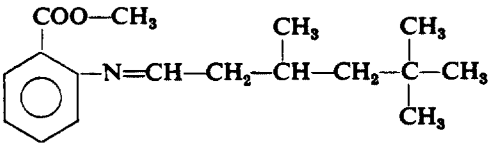
The lower homologue of this material is also known.

Prod.: from Trimethyl cyclopentadiene and Acetone by condensation.

(See also: 67-83).

## 2253: METHYL-N-(3,5,5-TRIMETHYLHEXYLIDENE)-ANTHRANILATE

*iso*-Nonylaldehyde Methylanthranilate.



$C_{17}H_{25}NO_2 = 275.40$

Yellowish viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Intensely sweet, floral-citrusy and tenacious odor with a "metallic-fresh" topnote. The odor may vary considerably according to the composition of the condensation product (or the ratio of the two components used).

This "Schiff's base" of an industrial aldehyde with Methylanthranilate has found a little use in perfume compositions, but since the base has not been offered commercially (it is generally made by the user himself) it has not achieved much popularity.

It could find use in low-cost fragrances for household articles, detergents, etc., but the character of the aldehyde is not commonly liked. It is a very powerful aldehyde, but its odor is typically "unnatural" and will rarely appeal to the "first-time-customer". The perfumer appreciates the power and the low cost – and the ability of the aldehyde to produce what is often called "ozone-like" odor complexes, desirable in many household products.

Prod.: from *3,5,5*-Trimethylhexaldehyde and Methylanthranilate by condensation under mild heat and progressive removal of water.

## 2254: METHYL TRISULFIDE

Dimethyl trisulfide.

$CH_3—S—S—S—CH_3$

$C_2H_6S_3 = 126.27$

Almost colorless or pale yellowish mobile oil.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Very powerful and diffusive, penetrating odor of fresh Onion, greener and more ethereal than the odor of the Methyl propyl trisulfide. The tenacity is extremely poor.

The title trisulfide, which has been identified in the volatile portion of fresh Onion juice, has been synthesized and is used in combination with other known components of the Onion flavor to re-constitute such flavor in processed food (vegetables, soups, etc.).

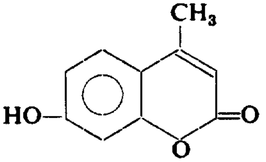
158-136;
(see also monograph: Methyl-*1*-propyl trisulfide).

## 2255: METHYL UMBELLIFERONE

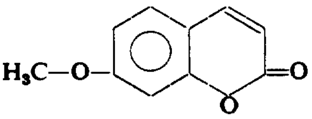
The perfumery literature is particularly confusing with respect to the nomenclature of this and related chemicals.

The monograph describes Umbelliferone methylether, or:
*7*-Methoxy coumarin.
Herniarin.
Ayapanin.

The chemical called *beta*-Methylumbelliferone, often confused with the title material, would be:
*4*-Methyl-*7*-hydroxycoumarin. It is a faintly coumarinic-smelling solid material, from which "Maraniol" (see *4*-Methyl-*7*-ethoxycoumarin) can be made. Umbelliferone itself (see monograph) is also odorous.



*4*-Methylumbelliferone.
*4*-Methyl-*7*-hydroxycoumarin.
M.P. 189° C.
Faintly coumarinic odor.
(Resocyanin).



Umbelliferone methylether. M.P. 118° C.
(Title material).
Virtually odorless.

$C_{10}H_8O_3 = 176.17$

White crystals.

Insoluble in water, poorly soluble in cold alcohol, slightly soluble in warm alcohol, soluble in certain oils.

This material – although practically odorless, is mentioned in the present work because it is an important material in Nature, and because it is often confused with the odorous empirical isomer.

Methylumbelliferone has no use in perfumes of flavors, but it has been used as a sunscreening agent. In fact, it has been suggested that Methylumbelliferone is one of the natural sunscreening agents in the tissue of certain plants, preventing deterioration of the delicate components of the essential oil which, under normal circumstances, would quickly decompose under sunlight.

Since Methylumbelliferone is practically non-volatile with steam, it will rarely be found in the essential oils, but it is present in certain absolute extracts (Lavender, etc.).

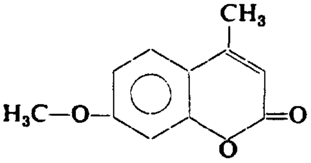
Prod.:
by Methylation of *7*-Hydroxycoumarin, which is obtained from

1) *2,4*-Dihydroxybenzaldehyde plus Acetic anhydride, or
2) Resorcinol (monomethylether) with Malonic acid and Sulfuric acid.

26-614; 61-70; 69-880; 90-600; 163-224; B-XVIII-31;

## 2256: METHYL UMBELLIFERONE METHYLETHER

*4*-Methyl-*7*-methoxycoumarin.
Resocyanin methylether.
Methoxyresocyanin.



$C_{11}H_{10}O_3 = 190.20$

White crystals.

Insoluble in water, poorly soluble in alcohol, soluble in some oils, almost insoluble in Propylene glycol.

Sweet-herbaceous, but very faint odor. When heated, the crystals emit a more pleasant nut-like or deep-caramellic sweetness of great tenacity. The odor is more coumarin-like and less Celery-like than that of the Maraniol (see monograph: *4*-Methyl-7-ethoxycoumarin).

This material has been suggested for use in perfume compositions, but is suffers from the same drawbacks as Maraniol: it is very poorly soluble in the conventional perfumery solvents, and it is not sufficiently powerful to compensate for this drawback.

Maraniol has survived, although it is surprisingly unknown to many perfumers, because it has a certain character and it is powerful enough to lend character to a fragrance composition in spite of its poor solubility.

The title material will probably disappear or fade into oblivion except for the perfumery research laboratory.

Prod.: from Resorcinol and Ethylacetoacetate, followed by Methylation with Dimethylsulfate in weak aqueous alkali.

103-303; (see also: 69-880). See also 2013;

## 2257: METHYL UNDECANOATE

Methyl undecylate.
Methyl hendecanoate.

$CH_3(CH_2)_9COO—CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless oily liquid. Sp.Gr. 0.88.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet, oily-winey, almost honeylike and tenacious odor.

Oily-Brandy-like, sweet taste in dilution. Fatty-fruity, not very pleasant at concentrations higher than 20 ppm.

This ester has found a little use in perfume compositions as part of "winey" topnote complexes with Cognac oil or Citrus complexes, etc. It supplies very pleasant notes in Rose and Lily.

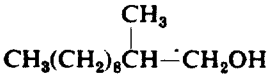
The subject material is also used to a minor degree in flavor compositions, mainly for imitation Cognac, Brandy, Rum, and in Banana.

Prod.: by direct esterification of Undecanoic acid with Methanol, preferably using azeotropic conditions.

103-81; 163-53;

## 2258: 2-METHYL UNDECANOL

*iso*-Lauryl alcohol.



$CH_3(CH_2)_8\overset{\overset{CH_3}{|}}{C}H-CH_2OH$

$C_{12}H_{26}O = 186.34$

Colorless oily liquid, solidifying in the cold.

Almost insoluble in water, soluble in alcohol and oils.

Very mild, "bland" odor of sweet-waxy, oily character, but not with the "fresh-laundry"-like odor of commercial Lauryl alcohol.

This alcohol is occasionally used in perfume compositions, mainly as a blender/modifier in delicate floral fragrance types (Lily, Rose, Peony, Freesia, etc.). It does not contribute much odor, but its natural-waxy effect is appreciated in those rare cases.

A number of isomers are also used in perfumery:

*3*-Methylundecanol-*3* and

*6*-Methylundecanol.

Prod.: from Methyl nonyl acetaldehyde by hydrogenation.

(See also: 163-363).

## 2259: METHYL-9-UNDECENOATE

Methyl undecylenate (Baker Chem. Co. Inc.).

$CH_3—CH{=}CH(CH_2)_7COO—CH_3$

$C_{12}H_{22}O_2 = 198.31$

Colorless or very pale straw-colored oily liquid.

Insoluble in water, soluble in alcohol and oils.

Light, fatty-green, mildly earthy-fungal odor with some resemblance to Brandy and Cognac.

Oily-brandy-like taste in concentrations below 50 ppm. Rather unpleasant "rubber-like" at higher concentrations.

This unsaturated ester is used to a limited extent in perfume compositions. It may supply interesting notes in Citrus topnote complexes and give pleasant variations in Cognac oil or other green-winey odors.

It is more frequently used, but normally in mere traces, in flavor compositions, such as Honey, Citrus, Rum, etc. It performs very well with Ethyl aceto acetate, Ethyl phenylacetate, Citronellyl acetate, Linalyl acetate, etc.

The concentration used is normally about 3 to 25 ppm in the finished product.

Prod.: by direct esterification of Undecylenic acid with Methanol. The acid may be obtained by pyrolysis of Castor oil (manufacture of Heptaldehyde and Undecenoic acid).

G.R.A.S. F.E.M.A. No.2750.

26-614; 100-1080; 163-224; 163-363; B-II-459;

## 2260: METHYL-n-UNDECIN CARBONATE

Methyl-*n*-undecyne carboxylate.
Methyl-*2*-dodecynoate.

$CH_3(CH_2)_8C{\equiv}C{-}COO{-}CH_3$

$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid.

Insoluble in water, poorly soluble in Propylene glycol, soluble in alcohol and oils.

Floral-waxy, mildly green, but not very "leafy" odor of considerable tenacity.

This ester is of very little interest to the creative perfumer. It is mentioned in this work for the sake of including "borderline" materials and to describe uncharacteristic members of the well known ester series.

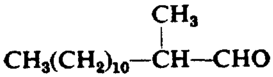
The title ester lacks natural character and foliage greenness, but it is pleasantly floral and waxy at proper dilution. Useful for certain floral fragrances, Narcissus, Lily, etc., but the perfumer does not really need this ester.

Prod.: from Decylbromide and Sodium acetylide via *2*-Undecyne sodium and with Methylchloroformate to the title ester.

7-272; 163-53; 163-224;

## 2261: METHYL UNDECYL ACETALDEHYDE

*iso*-Tetradecanal.
A C-14-aldehyde.



$$CH_3(CH_2)_{10}{-}\overset{\displaystyle CH_3}{\overset{|}{C}H}{-}CHO$$

$C_{14}H_{28}O = 212.38$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Mild-Ambre-like, semi-dry, waxy-resinous odor of good tenacity.

This aldehyde, rarely offered under its proper name, and not very commonly used, has occasionally been used in perfume compositions of the powdery-Ambre-like type, Oriental fragrances, etc.

It blends very well with the Ionones, Olibanum, Mimosa, Citrus and Cedarwood products, etc. and gives interesting nuances with Oakmoss and Spice oils.

Prod.: from Methyl undecylketone via Darzens synthesis with Ethyl monochloroacetate plus Sodium ethylate, followed by hydrolysis of the glycidic ester and heating of the acid under vacuum.

## 2262: METHYL UNDECYL KETONE

*2*-Tridecanone.
Hendecyl methyl ketone.

$CH_3{-}CO{-}(CH_2)_{10}CH_3$

$C_{13}H_{26}O = 198.35$

White waxy mass or colorless crystal leaves.
M.P. 30° C. Sp.Gr. 0.82 (liquid)
B.P. 263° C.

Insoluble in water, soluble in alcohol and oils.

Warm-oily, herbaceous or delicately spicy, nut-like odor of considerable tenacity.

Bland-oily taste, yet reminiscent of fresh Coconut meat.

This ketone finds a little use in perfume compositions as a modifier in sweet-floral and heavy-floral fragrance types, particularly as a companion to Nonanolide in Gardenia, etc. It gives pleasant effects in Citrus colognes and modern Fougères, and performs also well with Geranium, Coumarin etc.

The material is used in flavor compositions for imitation Coconut and other nut types, and in certain types of fruit-and-nut flavor for baked goods, where the tenacity of this ketone comes in useful.

Prod.:

1) by oxidation of Tridecanol-*2*.
2) from Lauric acid plus Acetic acid by heating over Thorium oxide at approximately 450° C.

26-614; 66-516; 89-176; 140-165; 160-1262; 163-224; 36-1144;

## 2263: METHYL VALERATE

Methyl-*n*-valerate.
Methyl pentanoate.
Methyl valerianate.

$CH_3—COO—(CH_2)_3—CH_3$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.89. B.P. 127° C.

Very slightly soluble in water, soluble in Propylene glycol, alcohol and oils.

Pungent-ethereal, green-fruity Apple-like odor of very poor tenacity. The odor is heavier than that of Methyl-*iso*-valerate (see next).

Sweet-ethereal Apple-like fruity-green taste in concentrations lower than 100 ppm.

This ester is primarily used in flavor compositions, although it occasionally finds application in certain phases of perfumery (masking, household products of certain type, etc.). Its Apple-like character is useful in fruit complexes where diffusive power is desirable (chewing gum, etc.) and it performs very well in Pineapple or fantasy flavors.

The concentration used is normally about 10 to 40 ppm in the finished product.

Prod.: by direct esterification of Methanol with *n*-Valeric acid e. g. under azeotropic conditions.

It should be kept in mind that this ester is very easily hydrolyzed, and that a chemically inert dehydrating agent such as anhydrous Sodium sulfate can be added to the stock bottle with good results. Needless to say that traces of free acid (Valeric) would be detrimental to the odor/flavor picture of the ester.

G.R.A.S. F.E.M.A. No.2752.

26-614; 33-932; 140-140; 160-1274; B-II-301; 163-225; 163-53;

## 2264: METHYL-iso-VALERATE

Methyl-*3*-methylbutanoate.
Methyl-*iso*-pentanoate.
Methyl-*iso*-valerianate.

$CH_3—OOC—CH_2—CH(CH_3)_2$

$C_6H_{12}O_2 = 116.16$

Colorless liquid. B.P. 117° C. Sp.Gr. 0.88.

Slightly soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Pungent,ethereal, fruity-Apple-like odor of poor tenacity.

Sharper than Methyl-*n*-valerate and, in some flavorists' opinion, less natural in character.

Sweet-ethereal and Apple-fruity taste (peel-like) in concentrations below 100 ppm. It seems less prone to decompose (and produce free acid) than the *n*-ester.

Again, this ester does find a little use in perfumery, and it has even been recommended for soap perfumes in conjunction with Ethyl butyrate, but the author would rather leave such comment as a "quote from literature" only.

The ester is mainly used in flavor compositions, often in the same places as described under the *n*-ester: Apple, fruit complexes, Pineapple, etc. and the concentration is normally about 10 to 35 ppm in the finished product.

Due to the better stability of the *iso*-valerate, there has been some interest on the part of the perfumers to find uses for this powerful odorant. Traces have been used in Geranium, and with Galbanum or Estragon it gives quite interesting effects. It should be used with utmost discretion, but it may, in the proper hands, produce novel and surprising effects in a fragrance.

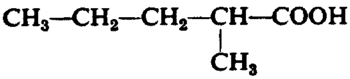
Prod.: by direct esterification of Methanol with *iso*-Valeric acid, preferably under azeotropic conditions.

G.R.A.S. F.E.M.A. No.2753.

(Sample: Fritzshe Bros. Co., Inc.).
26-614; 100-679; 103-81; 160-1068; 163-222; B-II-311;

## 2265: 2-METHYL VALERIC ACID

*alpha*-Methyl valeric acid.
*2*-Methylpentanoic-*1*-acid.
Methyl propyl acetic acid.
Pentane-*2*-carboxylic acid.



$$CH_3{-}CH_2{-}CH_2{-}\underset{\underset{\displaystyle CH_3}{|}}{CH}{-}COOH$$

$C_6H_{12}O_2 = 116.16$

Colorless liquid. Sp.Gr. 0.93. B.P. 194° C.

0.6% soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Powerful, pungent-acidulous odor, caramellic-sour. In extreme dilution pleasant oily-acidulous, herbaceous, but of poor tenacity.

In concentrations lower than 10 ppm the taste is pleasantly sour, oily, "dairy-product-like" with a mild or sweet aftertaste. Higher concentrations show pungency or bite and unpleasantly acid taste.

This acid finds some use in flavor compositions, particularly in imitation Cocoa and Chocolate, where the oily-acid note is quite appropriate. The concentration in finished products will usually amount to about 1 ppm – often less.

NOTE: Do not confuse this acid with *iso*-Caproic acid, which is *beta-iso*-Propylpropion-acid, or: *3*-Methylbutane-*1*-carboxylic acid.

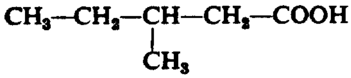
Another isomer, *beta*-Methylvaleric acid, or *2*-Methylbutane-*1*-carboxylic acid occurs naturally in tobacco leaves. See next monograph.

G.R.A.S. F.E.M.A. No.2754.

26-450; 66-571; 160-1274; B-II-326;

## 2266: 3-METHYL VALERIC ACID

*3*-Methylpentanoic-*1*-acid.
*secondary*-Butylacetic acid.
*beta*-Methylvaleric acid.
*2*-Methylbutane-*1*-carboxylic acid.
Exists in *dextro*- and *laevo*-forms, and in *dl*-form.



$$CH_3{-}CH_2{-}\underset{\underset{\displaystyle CH_3}{|}}{CH}{-}CH_2{-}COOH$$

$C_6H_{12}O_2 = 116.16$

Colorless liquid. Sp.Gr. 0.93. B.P. 196° C.

Soluble in water, miscible with alcohol and oils.

Sour-pungent odor, in dilution sour-herbaceous, slightly green, of poor tenacity.

In concentrations below 1 ppm the taste is warm-herbaceous, pleasantly sour, slightly green, and with a sweet aftertaste.

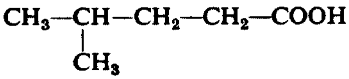
This acid has been synthesized since it was identified in tobacco leaves. It is used for reconstitution of tobacco flavor as part of a flavor complex.

The acid has been suggested for use in perfume compositions, but its chemical Nature is almost prohibitive for its use except in very minute proportions.

26-450; 66-571; 90-84; 160-1274; 163-363; B-II-331;

## 2267: 4-METHYL VALERIC ACID

*iso*-Caproic acid.
*iso*-Butylacetic acid.
*3*-Methylbutane-*1*-carboxylic acid.
*2*-Methylpentan-*5*-oic- acid.
*4*-Methylpentan-*1*-oic acid.



$$\mathrm{CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-CH_2-COOH}$$

$C_6H_{12}O_2 = 116.16$

Colorless oily liquid. Sp.Gr. 0.93.
B.P. 200° C.

Slightly soluble in water, soluble in Propylene glycol and alcohol, miscible with oils.

Unpleasant sour and penetrating odor. Less fatty-sweat-like than Caproic acid, more pungent.

The taste follows the odor picture except at very low concentrations where the sour taste is slightly fruity, no longer unpleasant.

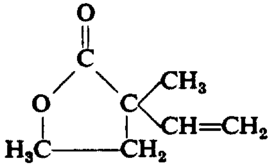
This acid, although identified in Nature, has found very little, if any, use in perfumes or flavors. It is mentioned mainly for the sake of completing the monographs on Methylpentanoic acids. It is rarely offered commercially, but may become a commercially available item if its esters become more interesting to the perfume and flavor industry.

Prod.: (66-573).

26-450; 90-83; 160-1058; B-II-327; 66-571; 157-210;

## 2268: gamma-METHYL-gamma-VINYL BUTYROLACTONE

An *iso*-Heptenyl lactone.



$C_7H_{10}O_2 = 126.16$

Colorless or very pale straw-colored oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and warm-herbaceous, oily-nut-like odor of moderate tenacity.

The title lactone which has been identified in Lavender and Lavandin oils and absolutes, has been synthesized and may find use in the reconstruction of these natural products.

The lactone represents an entirely new chemical group from Lavender and Lavandin, but the perfumer may not be so surprised if he is one of the alert workers who have already long ago tried *gamma*-Heptalactone as a Coumarin modifier in Lavender.

*gamma*-Octalactone is also used, but these materials are unfortunately still rather expensive even at the very modest concentration needed for the above purpose.

(See: American Perfumer & Cosmetics, vol. 83, April 1968, page 34).

## 2269: METHYL VINYL KETONE

Vinyl methyl ketone.
Methylene acetone.
*1*-Buten-*3*-one.

$CH_2{=}CH-CO-CH_3$

$C_4H_6O = 70.09$

Colorless mobile liquid. Polymerizes easily, loses odor, becomes practically insoluble in alcohol and most oils. B.P. 81° C.
Sp.Gr. 0.86.

Almost insoluble in water, soluble in alcohol and oils.

Very sharp and pungent, rather irritating and penetrating odor. In extreme dilution sweet-ethereal, not unpleasant.

This ketone has occasionally been used as an extraction solvent for natural raw materials to make oleoresins, concretes, etc.

It is briefly mentioned because it may be a trace impurity in the processed extract, and its odor will be perceptible if the material is relatively fresh.

As a solvent, it has the advantage of a boiling point very near that of alcohol, but since it is not miscible with water, it may be a better solvent for removal of water by azeotropic effect in the process of evaporation of the extract.

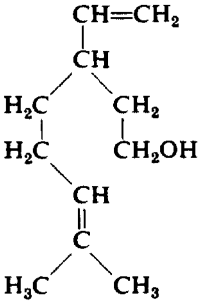
Prod.:

1) from Acetone and Paraformaldehyde.
2) by hydration of Monovinyl acetylene.

31-84; 66-531;

## 2270: 7-METHYL-3-VINYL-6-OCTEN-1-OL

"Methylene citronellol".



$C_{11}H_{20}O = 168.28$

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Mild, woody-floral, remotely rosy odor with some resemblance to Linalool or Ethyl linalool. Moderate tenacity.

The traces of camphoraceous-piney note, sometimes found in this material, may well be ascribed to impurities, but is does not help the material that such impurities may occur in the commercial product – which is sold under various trade names.

Unless this alcohol can be produced at a very attractive price – in other words come into volume production – there is not much future to see for the material, particularly in view of the wealth of chemicals available with similar type of odor.

Prod.: from Nopol via Dihydronopol and isomerization to the title material.

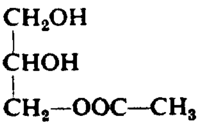
(See: American Perfumer & Cosmetics, vol. 83, April 1968, page 31).

## 2271: MONOACETIN

Acetin.

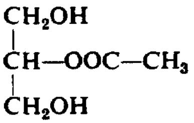
Glyceryl monoacetate.

The commercial product is a mixture of the two isomers:



$$\begin{array}{l} CH_2OH \\ | \\ CHOH \\ | \\ CH_2{-}OOC{-}CH_3 \end{array}$$

*1*-Monoacetin.



$$\begin{array}{l} CH_2OH \\ | \\ CH{-}OOC{-}CH_3 \\ | \\ CH_2OH \end{array}$$

*2*-Monoacetin.

$C_5H_{10}O_4 = 134,14$

The two isomers can be manufactured separately (see below). *2*-Monoacetin is more viscous. The monograph describes the commercial product (mixture).

Colorless or pale yellowish oily liquid.

Sp.Gr. 1.20. B.P. 257° C.

Miscible with water, alcohol, Propylene glycol and some oils, but only few. Insoluble in terpenes.

The material is hygroscopic and should be kept in well closed containers.

Faint, musty-sour odor, varying with the age and quality of the material. The commercial grade has almost always a sour note.

This ester is mentioned briefly because it has found some use as a flavor solvent (rarely as a perfume solvent).

It is not mentioned in the American Federal Register as G.R.A.S. or recognized by the F.E.M.A. Only the Triacetin (see monograph) is recognized for food use in the U.S.A.

Prod.: (all Acetins): from Glycerol and Acetic acid with Phosphoric acid catalyst.

(*1*-Mono-acetin, only): from *iso*-Propylideneglycerol plus Acetylchloride, followed by hydrolysis.

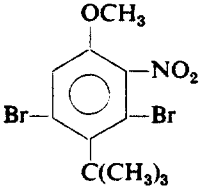
(*2*-Mono-acetin, only): from *1:3*-Benzylidene glycerol by acetylation with Acetic anhydride in Pyridine, followed by hydrogenation.

26-560; 66-1024; 100-688; 160-1014; B-II-146;

## 2272: MONONITRO DIBROMOBUTYL-meta-CRESOL METHYLETHER

*2*-Nitro-*3,5*-dibromo-*4*-*tertiary*-butylanisole. The literature occasionally refers to the non-nitrated product, and confusion with *4*-Bromo-*3*-methyl-*6*-*tertiary*-butylanisole also occurs.

The title material is mentioned only as one example of a halogenated, nitrated musk of benzene type.



$C_{11}H_{13}Br_2NO_3 = 367.07$

Pale yellowish crystals. M.P. 100° C.

Practically insoluble in water, poorly soluble in alcohol, soluble in certain oils, poorly in others.

Sweet Ambregris-musk-like odor of good tenacity.

The title material was patented in 1931 by a Swiss manufacturer, and it was at that time considered an interesting novelty. Brominated musks are, to the author's knowledge, no longer in use in perfumery, but they may serve as part of results obtained in chemical-olfactory research aimed at finding "musk-ophore" chemical groups, constellations, radicles, etc.

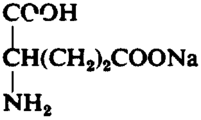
Musk chemicals of the benzene family including Chlorine, Iodine and Fluorine have also been manufactured, but are of little more than academic interest.

4-6; 4-43; 5-326; 7-34; 86-147; 156-272; 159-637; 163-4; 163-23; 163-103; 163-251; 4-201;

## 2273: MONOSODIUM GLUTAMATE

The sodium salt of (natural) *laevo-alpha*-Aminoglutaric acid.

The title material is known under a wealth of trade names, e. g.:
"Glutacyl", "Accent", "Zest", "Vetsin", "Glutavene", "M.S.G.", "RL-50", etc.
and is sometimes referred to as "Ajinomoto" (name of world's largest manufacturer, the name meaning "taste essence" in Japanese), Also called "Chinese Seasoning", etc.



$$\begin{array}{l}COOH\\ |\\ CH(CH_2)_2COONa\\ |\\ NH_2\end{array}$$

$C_5H_8NNaO_4 = 169.12$

White crystalline powder or small needles.

Soluble in water and alcohol, not in oils.

The commercial product usually has a faint, peptone-like odor, often simply called "meaty" or "soupy", but highly purified products show very little, if any, such odor.

A 1% solution in water has a sweet taste with a meat-like note.

This material is used exclusively as a food additive, not in perfumery. A French patent covers the use of Glutamic esters in perfumery claiming that these esters have odor-enhancing effect, parallel to the taste-enhancing effect of the title (water-soluble) material.

Monosodium glutamate is legally classified as a "food additive", not a flavor chemical. The material is very comprehensively described in food chemical literature (see below).

Monosodiumglutamate is used very extensively as an additive to flavor compositions, or as an additive directly to food.

It may be added at the rate of 1 ppm in candy to enhance the flavor (any flavor type), or it may be used at 4000 ppm in soups, condiments or meats. Certain observers may claim that 1 or 2 ppm is completely without any effect, and the question is still under debate as new and more powerful flavor enhancers or synergists are being developed and marketed.

The MSG is most often used in conjunction with Sodium chloride, and it may then be used at concentrations of up to 5000 ppm in the finished consumer product. The 5'nucleotides are used with salt and Monosodiumglutamate, thereby increasing the effect of MSG many times. Some of the "flavor potentiators" are mentioned in this work under the monographs Disodium guanylate and Disodium inosinate.

The history of Monosodium glutamate is relatively short. The material has been known since 1866 (as glutamic acid), but was not suggested as a flavor enhancer until 1908. Within 60 years, it has grown to become the greatest food chemical success of the century. The estimated world production for 1968 is 120,000 metric tons which is equivalent to 50 grams per year per person in the entire world.

The production in the United States of America is equivalent to 100 grams per U.S. citizen per year. And it is worthwhile noticing that one Japanese manufacturer produces about 3 times as much Monosodiumglutamate as all the American manufacturers combined.

Prod.:

1) by vegetable proteolysis of proteins.
2) from Molasses.
3) (synthetic) from Acrylonitrile. Exclusive Japanese process by Ajinomoto Co.

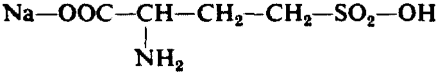
G.R.A.S. F.E.M.A. No.2756.

Now considered "a common food ingredient", and therefore so obvious in use, that it is no longer mentioned in the regular GRAS-list (U.S.A. 1968).

The Mono potassium glutamate and the Mono ammonium glutamate are also commonly used in food, and classified as G.R.A.S. by the American F.D.A. (162-671).

100-1115; 157-516; 158-262; 158-264; 159-670; 162-495;
see also: Chemical & Engineering News, October 10, 1966, pages 129-130.

## 2274: MONOSODIUM-l-HOMOCYSTEINATE



$Na{-}OOC{-}\underset{NH_2}{\underset{|}{CH}}{-}CH_2{-}CH_2{-}SO_2{-}OH$

$C_4H_9NNaO_5S = 206.18$

White crystalline powder.

Practically odorless. Very little taste of its own, even at concentrations higher than suggested use-concentration.

This material is suggested as a flavor enhancer and synergist, sometimes called a "flavor potentiator" to be used in conjunction with Monosodium glutamate and the 5'nucleotides.

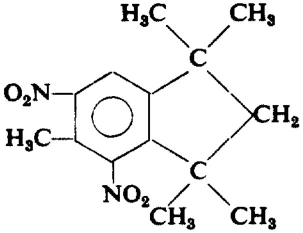
The salt is to be used in food seasoning.

Its manufacture is covered by a Japanese patent (pending since Sept. 1966) owned by the Ajinomoto Company, also the world's largest manufacturer of Monosodium glutamate.

See also: 157-516/532, and 158-261/273;

## 2275: MOSKENE

*1,1,3,3,5*-Pentamethyl-*4,6*-dinitroindan.
The title name is the trade name used by Givaudan Corp.



$C_{14}H_{18}N_2O_4 = 280.33$

Pale yellowish or whitish-ivory-colored crystals or crystalline powder. M.P. 132° C.

Almost insoluble in water, 1% soluble in alcohol, 17% soluble in Benzylbenzoate, 24% soluble in Diethylphthalate at room temperature.

Musky-sweet odor of type resembling Musk Ketone and Musk Ambrette, yet more creamy-floral, sweeter and more tenacious.

This Nitro-indan musk represents the transition from the original Benzene-Nitro-musks to the Indan-type musks, most of which are non-nitrated.

The material was an almost immediate success, and has grown to become a large-volume, low-cost everyday-use musk in an amazingly short time (in perfume chemical terms).

It has the advantage of being much less sensitive to sunlight than the "three old Nitromusks", yet being a low-cost, oil-soluble, all-purpose musk.

Its soft and sweet odor helps introduce the very desirable "creamy" powdernote for various types of cosmetic fragrance, and it performs particularly well with the Methylionones for such purpose.

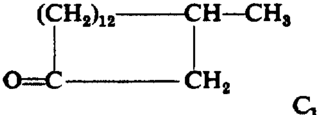
Prod.:

1) from *para*-Cymene plus *iso*-Butene, followed by Nitration.
2) from Toluene plus Mesityloxide via the carbinol to the tertiary alcohol, then cyclization and Nitration.

106-268; 156-269; 156-279;
see also: T.Wood: special Musk reports, "Givaudanian", Jan. 1968 ff.,
and: Carpenter (Givaudan): Polycyclic Musks (1955 report).

## 2276: MUSCONE

*3*-Methylcyclopentadecanone-*1*.
*laevo*-Muscone.
*beta*-Methylcyclopentadecanone-*1*.
Methylexaltone.
This monograph includes:
*racemic*-Muscone, or
*dl*-Muscone.



$C_{16}H_{30}O = 238.42$

White or colorless or opaque crystalline mass, M.P. 33° C. When supercooled, it is a liquid, colorless and viscous. Sp.Gr. 0.92. The boiling point is higher than 300° C. (328° C. – extrapolated).

Almost insoluble in water, soluble in alcohol and oils.

Very soft, sweet and extremely tenacious, musky, but not animal, odor. The power is only fully realized when the material is diluted. An alcoholic solution containing 0.1% Muscone smells strongly of the material, not of alcohol. This is typical of the truly superior fixatives, including Exaltolide and Ambrettolide, and several of the new Oxalactone-musks.

Natural Muscone is *laevo*-Muscone, while synthetic Muscone is *racemic*- or *dl*-Muscone. 14 grams of Muscone equals the Muscone content in one kilo of natural musk grains. Needless to add that Muscone does not constitute the entire odor or fragrance power of natural musk, but if Musk Tincture is used mainly for its tenacity, this part of its action can be replaced by a certain amount of Muscone. The cost of fixation is considerably reduced by this replacement, since synthetic Muscone costs less than natural musk grains (approximate market price Sept. 1968 = U.S. $ 5,000,– per kilo), and the amount of Muscone needed is 50 to 75 times less than that of Musk grains. However, the perfumer, experienced in the use of Musk Tincture, will undoubtedly agree, that the exchange proportion is not quite so favourable to Muscone as the calculated figures may indicate. Such experience resemble the findings when the flavourist tries to replace Vanilla tincture with Vanillin.

Although Muscone is non-existing in many perfume laboratories, it is used discretely in a large number of fine perfumes. It takes considerable experimenting and time-consuming study of the finished (functional) products to fully estimate the effect of Muscone in a fragrance. It performs best when the perfumed product is applied to the human skin, and is therefore mainly found in luxury perfumes, powder perfumes, creme perfumes, etc., but rarely in bathoils, etc.

Prod.: – numerous patented methods which could be classified in

A: from inexpensive raw materials but giving poor yields.

B: from expensive starting materials, giving high yields.

e.g.:

1) from Glycols, via dicarboxylic acids.
2) from Dinitriles by cyclization.
3) from Diketones by cyclization, etc., etc.

The formation of *laevo*-Muscone from Stearic acid by biogenesis (in natura) is considered probable.

4-89; 5-194; 5-195; 31-100; 31-101; 31-107; 67-280; 100-696; 26-616; 156-256; 159-632; 163-55; 163-226; 163-364; B-VII-51-zweiter Ergänzungsband.

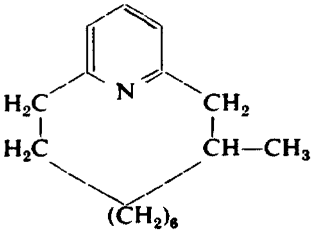
The human nose is notoriously poor in judging strength of powerful musks, and in discriminating between closely related macrocyclic musks. The synthetic Muscone is considered almost equal to the natural (*laevo*-) Muscone with respect to strength and performance.

See also monographs:

*1*-Methylcyclopentadecan-*2*-one.
*4*-Methylcyclopentadecan-*1*-one.
*5*-Methylcyclopentadecan-*1*-one.

## 2277: MUSCOPYRIDINE

*dextro*-Muscopyridine.



$C_{16}H_{25}N = 231.38$

Colorless or very pale straw-colored viscous liquid. Solidifies in the cold to an opaque crystalline mass. B.P. 264° C.

Very slightly soluble in water, soluble in alcohol and oils.

This material, which has been identified in natural musk grains, is considered part-responsible for the Urine-ammoniacal odor, characteristic of the topnote of (fresh) musk grains.

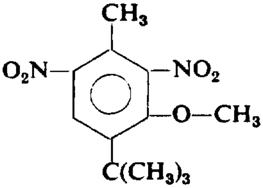
It is mentioned briefly in this work because the author believes that this (and several other) materials, identified in rare or expensive natural materials, may be classified as more or less "undesirable". A tendency toward the reconstitution of natural materials by synthetic means, but omitting the materials which may be classified as olfactorily undesirable, is pictured in certain new products, and the author would not only welcome this new development, but also predict a good future for the idea.

The title material has been synthesized, but the author has no personal report or sample of the material from any commercial supplier.

34-578; 86-102; 163-226; 163-364;
see also: Journal of the American Chemical Society, vol. 79, 1957, page 5558).

## 2278: MUSK AMBRETTE

*2,6*-Dinitro-*3*-methoxy-*1*-methyl-*4*-*tertiary*-butylbenzene.
*6*-*tertiary*-butyl-*3*-methyl-*2,4*-dinitroanisole.
*2,4*-Dinitro-*3*-methyl-*6*-*tertiary*-butylanisole.
*2,6*-Dinitro-*3*-methoxy-*6*-*tertiary*-butyltoluene.
*4*-Methoxy-*1,3*-dinitro-*2*-methyl-*5*-*tertiary*-butylbenzene.



$C_{12}H_{16}N_2O_5 = 268.27$

Pale yellowish or whitish-yellow or yellow crystals (varying with crystal size and structure). M.P. 83° C.

Almost insoluble in water, 3.3% soluble in alcohol, 37% soluble in Diethylphthalate, 50% soluble in Benzylbenzoate, practically insoluble in Terpenes or mineral oil.

Sweet, yet heavy, floral-musky odor of very good tenacity. The characteristic note of this Nitromusk is the floral tone of its muskiness.

The taste is bitter except in very low concentrations – best at 1 ppm or lower, unless powerful sweetening flavor materials are added (Cassia oil, Undecanolide, etc.). The effect is then sweet and musky at a discrete level.

Musk Ambrette is one of the most frequently used artificial musks. It is hard to imagine a day's work unless the jar with Musk Ambrette has been used. Many perfumers use it – almost conventionally – with Musk Ketone, generally favouring the Musk Ketone in proportion, to achieve part of the always desirable "powder" note in a fragrance.

The concentration of this material in a perfume formulation may be as low as 1% or as high as 15%, in rare cases even higher. One successful Cologne for Men a few years ago surprised many perfumers when it became evident that it contained about 12% combined Nitromusks, which is several times the conventional level (prior to that type Cologne).

In general, Musk Ambrette is a fixative, forming part of the "crystals" in a perfume formulation with other musks, Heliotropine, Coumarin, etc. It performs very well with the Ionones and with all members of the Linalool family, with Hydroxycitronellal or the Cinnamic alcohol group, etc., etc.

Among its minor drawbacks is the discoloration under daylight. This disadvantage has been greatly diminished as modern technique has supplied us with much purer Nitromusks. Apparently, the impurities were more sensitive, or they enhanced the photosensitivity of the musk itself. And modern soaps are so much better than those of 10-30 years ago, that discoloration due to incorporation in soap has been reduced or eliminated for many perfume chemicals, earlier considered as "troublemakers" in soap perfumes.

Musk Ambrette is used to a minor degree in flavor compositions.

It finds its way into such types as Cherry, Maple, Nut, Spice, Vanilla, Mint, Fruit, etc. and has been used in trace amounts in dentifrice flavors. Overdosage may easily cause a "perfumey" taste in such products.

The normal concentration in the finished product is about 0.01 to 10 ppm (a very wide range of concentrations), but the average is about 1 ppm. For certain old-fashioned types of licorice flavor ("Sen-Sen" and similar type) the concentration may be considerably higher.

Prod.: from *meta*-Cresolmethylether with *iso*-Butylchloride (or *iso*-Butylene) followed by Nitration of the ether.

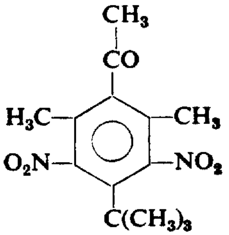
G.R.A.S. F.E.M.A. No.2758.

NOTE: Musk Ambrette is the only Nitromusk recognized as safe for food flavors in the U.S.A.

5-300; 7-290; 27-223; 29-317; 30-429; 31-194; 61-269; 86-100; 95-200; 96-226; 106-269; 156-278; 159-634;

## 2279: MUSK KETONE

*2,6*-Dinitro-*3,5*-dimethyl-*4*-acetyl-*tertiary*-butylbenzene.
*2,6*-Dimethyl-*3,5*-dinitro-*4*-*tertiary*-butylacetophenone.
*4*-*tertiary*-Butyl-*3,5*-dinitro-*2,6*-dimethylacetophenone.



$C_{14}H_{18}N_2O_5 = 294.30$

Pale yellowish platelets or crystalline powder. M.P. 137° C.

Practically insoluble in water, poorly soluble in alcohol, soluble in Diethylphthalate, Benzylbenzoate and most other perfume solvents, but not in terpenes, mineral oil or Propylene glycol.

Sweet and very tenacious musky odor with discrete animal note, less floral than Musk Ambrette. The characteristic note is the warm and mildly animal note.

Sweet and mildly musky taste in concentrations lower than 40 ppm. Musk Ketone has less tendency of producing a bitter note than Musk Ambrette. Yet, Musk Ketone is not listed as G.R.A.S. by the American Federal Register.

Musk Ketone is, with Ambrette and Xylol, one of the most frequently and widely used artificial musks. It is used in perfume compositions often in conjunction with Musk Ambrette as part of the fixative complex for almost any fragrance type. However, it is particularly suitable for producing the desirable "powdery" note with Methylionones, Cinnamic alcohol, Benzylsalicylate, etc. Concentrations vary from about 1% to more than 10% (in rare cases) in the fragrance formulation.

Musk Ketone discolors under daylight, but will normally not cause any significant discoloration in a soap at reasonable use-level. It forms adducts with Anthranilates and may discolor in the presence of Indole or other perfumery amines.

The title material has been used in flavor compositions at concentrations up to 20-45 ppm (in the finished product), mainly as a fixative and sweetener in chewing gums and other types of candy. The material is included in the "Chemicals Used in Food Processing" by the National Research Council, Washington, DC, 1965, but Musk Ketone is *not* listed as G.R.A.S. in the latest summary of the F.E.M.A. or the Federal Register.

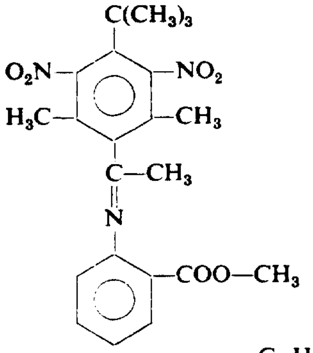
Prod.: from *tertiary*-Butylxylene by Acetylation followed by Nitration.

3-86; 5-299; 7-290; 27-224; 29-304; 30-428; 31-194; 95-200; 96-228; 106-270; 156-277; 163-225;

## 2280: MUSK KETONE - METHYLANTHRANILATE

An ill-defined, incomplete product.

The structure below represents a theoretical structure of the completed adduct.



$C_{22}H_{25}N_3O_6 = 427.47$

Viscous, yellowish or pale orange-colored liquid.

Insoluble in water, soluble in alcohol and oils.

Intensely sweet, floral-musky odor with variable notes of one or the other component, according to origin of the material, and method of manufacture.*

This "Schiff's base" type material was developed when certain adducts became popular in perfumery. Only a few have remained of considerable interest, and among them very few adducts with Ketone components.

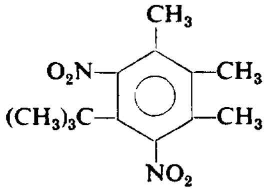
It is not uncommon that Musk Ketone and Methylanthranilate will occur in the same fragrance composition, and all indications point at that the use of the two materials separately will give satisfactory results, not improved by the use of an ill-defined adduct.

The title material is briefly mentioned in this work as an example of a "condensation product" with Methylanthranilate of very little, if any interest to the creative perfumer, but of some interest to the academic study of "Schiff's bases", etc.

33-1029; see also: 103-163;

## 2281: MUSK TIBETENE

*5-tertiary*-Butyl-*4,6*-dinitrohemimellitene.
*2,6*-Dinitro-*3,4,5*-trimethyl-*tertiary*-butylbenzene.
*5-tertiary*-Butyl-*1,2,3*-trimethyl-*4,6*-dinitrobenzene.



$C_{13}H_{18}N_2O_4 = 266.30$

Pale yellowish crystals or yellowish-whitish crystalline powder. M.P. 136° C.

Practically insoluble in water, 1.4% soluble in alcohol, 14% soluble in Diethylphthalate, 27% soluble in Benzylbenzoate. Sufficiently soluble in most perfume materials, except in Terpenes and other hydrocarbons. Almost insoluble in Propylene glycol and Glycerin.

Delicately sweet-musky, mildly, but unquestionably animal-like and very tenacious odor.

This Nitromusk represents one of the most successful improvements of the three "classical" musks. The title material has the advantage of being stable under exposure to daylight, yet it has the odor characteristics of Musk Ketone, perhaps slightly more delicately animal and sweet. This musk is used on a large scale even today with strong competition from non-nitrous musks. But Musk Tibetene maintains its popularity at a price level very near that of the two "old" Nitromusks (Ketone and Ambrette). It contributes pleasant and lasting undertones in powdery-floral and Oriental fragrances, in Colognes and soap perfumes, etc.

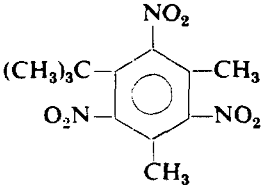
The subject Nitromusk is not permitted in food flavors in the U.S.A.

Prod.: from *meta*-Xylene via its *tertiary*-Butylderivative, followed by treatment with Formaldehyde and hydrochloric acid, reduction and Nitration to title material.

106-271; 156-271; 163-55; 163-226;
see also: T.F.Wood: Nitromusks, in the "Givaudanian", January 1968.

## 2282: MUSK XYLOL

Musk Xylene.
Xylolmoskus.
Musc Xylol.
*5-tertiary*-Butyl-*2,4,6*-trinitro-*meta*-xylene.
*2,4,6*-Trinitro-*5-tertiary*-butyl-*meta*-xylene.
*1,3,5*-Trinitro-*2-tertiary*-butylxylene.
*2,4,6*-Trinitro-*1,3*-dimethyl-*5-tertiary*-butylbenzene.



$C_{12}H_{15}N_3O_6 = 297.27$

Pale yellowish crystals or fine crystalline powder. M.P. 114° C.

Insoluble in water, slightly soluble in alcohol, soluble in most perfume oils, but very poorly soluble in Terpenes and other hydrocarbons, in Propylene glycol and Glycerin.

Sweet-musky and tenacious odor, rather harsh in its initial approach. This musk imparts sweetness but lacks the softness, floral or animal tonalities and overall power of the other Nitromusks.

Musk Xylol is sensitive to daylight, but it can be used in soap perfumes at normal concentrations (about 3 to 6% in the perfume composition). It does not replace Musk Ketone or Musk Ambrette weight for weight, but at least twice the amount of Musk Xylol is required to achieve a similar effect. The price of Musk Xylol is less than one-third of the Musk Ambrette or -Ketone prices.

Musk Xylol is also sensitive to Amines, particularly to Indole, with which it may develop a reddish color, even at normal use-concentrations in a perfume composition.

It is used very widely in all types of low-cost and ordinary fragrances for household products, for industrial purposes, inexpensive cosmetic products, etc. and it is very often accompanied by Amylsalicylate and Coumarin, Lavandin oil or Citrus oils, or it is the main fixative in a Pine fragrance, etc.

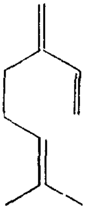
Musk Xylol can *not* be used in flavors in the USA.

Prod.: from Xylol with *iso*-Butylene (or *iso*-Butylchloride) via *tertjary*-Butylxylene and by Nitration to the title material. The process is considered relatively hazardous, and many explosions have occurred in the manufacture of this chemical, so closely related to TNT (Trinitro toluene, an explosive).

5-298; 26-710; 95-199; 96-225; 100-696; 106-272; 156-277; 159-633; 160-1104; 163-54; 163-225; B-V-448;

## 2283: MYRCENE

*7*-Methyl-*3*-methylene-*1,6*-octadiene.
Commercial grades of this material may contain up to 20 or 25% *laevo*-Limonene plus minor amounts of *beta*-Pinene and polymers.



$C_{10}H_{16} = 136.24$

Colorless or very pale straw-colored mobile liquid. It may acquire a pale amber color and it may eventually resinify (polymerize) upon exposure to daylight and air.

B.P. 167° C. Sp.Gr. 0.79 (pure material).

Insoluble in water, soluble in alcohol, miscible with most perfume oils.

Sweet-balsamic-resinous "gum" odor of poor tenacity. The odor of the purified Myrcene is refreshing, almost citrusy, but warm-balsamic, and ethereal-sweet.

The taste is sweet-balsamic-herbaceous at concentrations below 10 ppm. Higher concentrations tend to give pungency, bitterness or "gassy" taste.

This terpene finds use in perfume formulations where its spicy-balsamic and refreshingly light character introduces desirable notes in Citrus and spice colognes (an excellent extender of the odor of Bay leaf oil), or it finds more extensive use in masking odors for industrial purposes, mainly because of its low cost. It is also used as component of artificial essential oils, and as a fresh note in common household products.

The use as such in perfume compositions is, however, only a drop in the oceanvolume of Myrcene manufactured as an intermediate in the production of Terpenealcohols, Citral, Ionones, Hydroxycitronellal, etc.

Trace amounts of Myrcene are used in flavor compositions such as "root-beer", Citrus, Coriander, fruit-complexes, etc. The concentration in the finished product will normally be from 0.5 to 5 ppm.

G.R.A.S. F.E.M.A. No.2762.

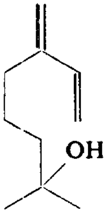
Prod.: by thermal isomerization of *beta*-Pinene (pyrolysis).

31-5; 67-494; 87-30; 100-699; 163-55; 163-226; 163-364; (The Glidden Co., Div. of SCM Corp. data sheet, May 1961: Myrcene "85").

## 2284: MYRCENOL

*2*-Methyl-*6*-methylene-*7*-octen-*2*-ol.
*3*-Methylene-*7*-methyl-*1*-octen-*7*-ol.

The commercial material will normally contain significant amounts of *alpha*-Terpineol and other alcohols.



$C_{10}H_{18}O = 154.25$

Colorless viscous liquid. B.P. 213° C.
Sp.Gr. 0.89.

Tends to polymerize on standing, increases in viscosity, decreases in odor power.

Practically insoluble in water, soluble in alcohol and oils.

Fresh, floral-Lime-like odor of moderate to poor tenacity. The Lime note is inevitably accompanied by woody notes, but should not show "piney" notes ("other alcohols").

Although this material has an unquestionably interesting odor, its drawback of poor shelf-stability has limited its use and popularity very strictly. Even its esters, the acetate in particular, have a limited shelf-life, unless very carefully kept under Nitrogen-blanket and a steady, cool temperature. Inhibitors may be added and they can have some improving effect.

Strange as it may seem to the perfumer or non-chemist, the alcohol made from the much less stable terpene Ocimene, an isomer of Myrcene, has gained popularity and seems to be fairly stable in the commercial grade. However, Ocimene and the Ocimenyl esters are much more expensive than the Myrcene members.

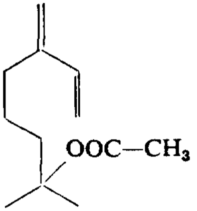
Myrcenol is used in perfume compositions for "lift" and freshness in floral or citrusy and "light" compositions, including soap perfumes. The Dihydromyrcenol is probably more popular as Lime-material, while Tetrahydro myrcenol is milder (weaker) and more floral. The latter material forms part of the commercial product known as Tetrahydromuguol (I.F. & F.).

Prod.: by chlorination of Myrcene, followed by hydrolysis.

156-374; (I.F.F.-material).

## 2285: MYRCENYL ACETATE

*3*-Methylene-7-methyl-*1*-octen-7-yl acetate.
*2*-Methyl-*6*-methylene-7-octen-*2*-yl acetate.
The commercial material contains acetates of related alcohols.



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. B.P. 224° C.

Insoluble in water, soluble in alcohol and oils.

Fresh, diffusive, sweet citrusy-herbaceous odor of moderate to poor tenacity.

This ester has found some use in perfumery as a modifier in Lavender fragrances, and as a blender in Citrus fragrances. It gives very interesting effects with Styrax products, with Patchouli and Bergamot in "Oriental" types, and it is also used in artificial essential oils.

Myrcenyl acetate is a major component of the product known as Pseudo Linalyl Acetate (I.F.F.) or "Neobergamate" (Naarden) and other specialties. These specialties are extremely complex mixtures from a reaction involving Myrcene and Acetic anhydride. The complex was manufactured long before Myrcenyl acetate became a commercial article, and it gained popularity by its unusual strength, justifying a price which is even higher than that of Linalylacetate. The strength and stability in soap made "Pseudolinalylacetate" (see monograph) popular as if it were an essential oil, and it was almost as complex.

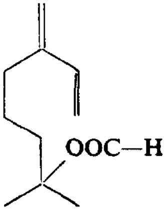
Myrcenyl acetate has in proper dilution a very pleasant Pear-like aroma (and taste), but the Propionate (see next) is even more pleasant.

Prod.: by cold Acetylation of Myrcenol. The yield is fractionated.

156-374; (I.F.F.-material).

## 2286: MYRCENYL FORMATE

*3*-Methylene-7-methyl-*1*-octen-7-yl formate.
*2*-Methyl-*6*-methylene-7-octen-*2*-yl formate.
The commercial product contains related esters and alcohols.



$C_{11}H_{18}O_2 = 182.27$

Colorless mobile liquid. B.P. 207° C.

Almost insoluble in water, soluble in alcohol and oils.

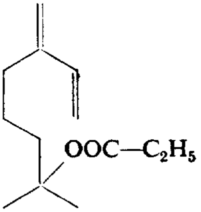
Fresh, green-citrusy odor with some resemblance to topnotes of Clary Sage oil. Moderate to poor tenacity.

This ester finds limited use in perfumery, mainly as a modifier in citrusy Cologne type fragrances, where it will support Bergamot, Petitgrain, Rosemary, Lavender and similar oils, and it will exercise its effect in the topnote only. In proper blends with alifatic aldehydes, it may produce very refreshing notes and pleasant sweetness, covering the chemical pungency of the aldehydes.

Prod.: by azeotropic esterification of Myrcenol with Acetic-Formic acid.

## 2287: MYRCENYL PROPIONATE

*3*-Methylene-7-methyl-*1*-octen-*1*-yl propionate.
*2*-Methyl-*6*-methylene-*7*-octen-*2*-yl propionate.
The commercial product contains small amounts of related esters.



$C_{13}H_{22}O_2 = 210.32$

Colorless liquid. Almost insoluble in water, soluble in alcohol and oils. B.P. 234° C.

Sweet and fruity-balsamic odor with a mild citrus note. The odor has striking resemblance to that of "canned pears", and some observers even claim that they find the "metallic" note in it.

This ester was developed after the apparent success of Pseudo Linalyl acetate and later Myrcenyl acetate. The title ester is somewhat more stable than the acetate, and it offers a very interesting tool in Bergamot compositions. It blends exceptionally well with the natural oil, has almost the same volatility, and simply enriches the oil.

For citrus variations, for Lavender compositions, and with Styrax in Oriental bases, it gives new and pleasant effects.

Due to its chemical structure it is not completely safe from polymerization, but its keeping qualities are satisfactory under normal storage and compounding conditions.

Although not listed specifically as "free" to use in flavors, it could be an interesting item in "Tutti-frutti" and in Pear and Mango imitation flavors.

Prod.: from Myrcenol and Propionic anhydride at regulated temperature and fractionation of the reaction distillate.

I.F.& F. material.

## 2288: MYRISTIC ACID

Tetradecanoic acid.
Tridecancarboxylic acid.
This acid is the chief component of Orris concrete oil ("Orris butter").

$CH_3(CH_2)_{12}COOH$

$C_{14}H_{28}O_2 = 228.38$

Colorless leafy crystals. M.P. 54° C.
Sp.Gr. 0.86 (liquid). B.P. 326° C.

Insoluble in water. Soluble (45%) in alcohol. Soluble in some, but not all oils. Practically insoluble in Propylene glycol and Glycerin.

Very faint, waxy-oily odor, almost odorless when pure, but since the commercial material is often contaminated with traces of unsaturated acids, etc., an acid-rancid or acrid odor may occur in older material.

The taste is bland, waxy at concentrations around 10 ppm, but pure material is practically tasteless (at least below that level). It produces a waxy mouthfeel which, in combination with organoleptically active ingredients may alter the overall flavor in an attractive manner.

The acid finds some use in perfumery e.g. as component of artificial Orris (concrete) oil. It has also been used in Mimosa compositions, and as a simple "cutting" agent of various essential oils, flower absolutes, etc. Myristic acid is used in trace amounts in imitation Butter flavor, in Butterscotch, Chocolate, Cocoa, fruit complexes, etc.

The concentration is normally as low as 0.1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2764.

Prod.: from the fatty acid mixture of Palm seed oil, or from Spermwhale oil.

26-616; 90-102; 100-700; 160-1104; 163-55; 163-226; B-II-365.

## 2289: MYRISTIC ALCOHOL

Myristyl alcohol.
Alcohol C-14 (true).
*l*-Tetradecanol.

$CH_3(CH_2)_{12}CH_2OH$

$C_{14}H_{30}O = 214.39$

Colorless or opaque waxy mass or leafy crystals. M.P. 41° C. Sp.Gr. 0.82 (liquid). B.P. 286° C.

Soluble in alcohol and oils, poorly soluble in diluted alcohol, insoluble in water, Propylene glycol, Glycerin.

Very faint, Coconut-oily, mildly waxy odor of considerable tenacity. A highly purified product is almost odorless.

This alcohol is rarely used in perfumes for olfactory purposes, but it finds extensive use in cosmetic preparations as an emollient. If the Myristic alcohol is not of high grade, there will be a problem of compensating for the odor of that ingredient, since the amount of Myristic alcohol in the cosmetic product will be many times higher than that of perfume.

This could be said of every single material that goes into a cosmetic preparation, and the problem is one with which the perfumer is very often faced and has great trouble explaining to the customer (or the cosmetic manufacturer). In fact, certain cosmetically desirable components may have such repulsive odors that the perfume must be specifically created "around" them, thereby limiting the choice of fragrance type very strictly.

Prod.: from the head oil of the Sperm Whale via the acid and the ester.

100-700; 106-273; 163-55; 163-226; B-I-428;

## 2290: MYRISTIC ALDEHYDE

Tetradecanal.
Myristaldehyde.
Tetradecyl aldehyde.
Aldehyde C-14 (true).

$CH_3(CH_2)_{12}CHO$

$C_{14}H_{28}O = 212.37$

Colorless liquid. Sp.Gr. 0.84. B.P. 260° C.

Polymerizes easily and solidifies into a whitish amorphous mass, melting af 65° C.

The aldehyde itself will solidify in the cold to an opaque mass which melts at 23° C. (non-polymerized).

Very faint, fruity-citrusy odor with an Ambre-incense note, somewhat dry and moderately tenacious.

This aldehyde finds some use in perfumery for its refreshing effect upon Citrus notes ("peel-effect"), and its pleasant refreshing lift to Olibanum (it takes the "touch-of-Pine" out of Olibanum).

It is also used frequently in combination with the Methylionones for Orris notes, and to reduce an overly sweet tone in certain fruity fragrance types. The combination with Undecanolide ("so-called aldehyde C-14") is quite interesting.

Traces of this aldehyde may introduce very pleasant notes in sophisticated Pine needle fragrances, and in modern versions of Chypre or "aldehydic" compositions.

The title aldehyde finds a little use in flavor compositions, mainly in Citrus (for the "peel"-effect), fruit complexes, and in imitation Honey. The concentration used is about 0.1 to 3 ppm in the finished product.

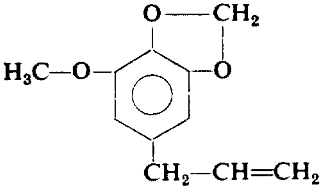
Prod.: by catalytic oxidation of Myristic alcohol.

G.R.A.S. F.E.M.A. No.2763.

41-37; 89-34; 106-40; 128-240; 140-159; 163-226; 163-55; B-I-716;

## 2291: MYRISTICIN

*4*-Allyl-*6*-methoxy-*1,2*-methylenedioxybenzene.
*3*-Methoxy-*4,5*-methylenedioxyallylbenzene.
*5*-Methoxysafrole.



$C_{11}H_{12}O_3 = 192.22$

Pale yellowish or almost colorless oily liquid. Sp.Gr. 1.14. B.P. 250° C.

Almost insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Pleasant and warm-balsamic, slightly woody odor of good tenacity. The undiluted material shows some "pepperiness".

This material, although commonly found in natural oils, has found only limited use in perfumery. As a component of artificial essential oils, and as a modifier in modern spice blends, etc.

One reason might be that it has not been manufactured synthetically at an attractive price. Attractive would mean "competitive with Eugenol" in this case. And, since any reasonable synthesis for Myristicin would start from Eugenol or a Eugenolderivative (except the Catechol synthesis), the synthetic Myristicin would never be made at a cost lower than Eugenol.

There is a possibility of extracting the Myristicin from an essential oil consisting primarily of that ether (Peruvian Clavel Moena leaf oil). The content in Nutmeg oil is too small to be of interest as such. The toxicity of Myristicin has been the center of much attraction, and the suspicion that Nutmeg (and Mace) present a hazard to the human digestive (or Central Nervous) system has been the subject of much discussion. If the unsaturated side-chain is responsible (and not the Methylenedioxy-ring), then we would be justified in assuming that Safrole, Eugenol and many related spice chemicals would be equally hazardous. The narcotic effect of Nutmeg has repeatedly been brought up in literature, and cases of using Nutmeg as a "dope" or "narcotic drug" are facts. Needless to add, that Myristicin is *not* permitted in food flavors in the USA (or in most other countries).

Prod.:

1) by isolation from various essential oils, including certain varieties of Ocimum species, or from Peruvian Clavel Moena oil.
2) from Catechol monomethylether via the Methylallyl ether.
3) from Eugenol via *5*-Hydroxyeugenol.

31-147; 68-978; 85-88; 90-473; 104-177; 104-445; 160-1104;

## 2292: MYRISTIC NITRILE

Tridecyl cyanide.
Tetradecyl nitrile.

$CH_3(CH_2)_{12}CN$

$C_{14}H_{27}N = 209.38$

Sp.Gr. 0.83. B.P. 286° C.

Colorless liquid. Solidifies in the cold, melts at 19° C. Almost insoluble in water, soluble in alcohol and oils.

Very powerful, in dilution refreshingly citrusy, in concentration rather choking, pungent odor of considerable tenacity, and with an undertone of fresh Oakmoss.

This Nitrile was one of the pioneering materials in what eventually became a new range of perfume chemicals.

It was developed by one of the most versatile perfume chemists and engineers of this century: Dr. Georges Igolen, then Technical Director at Antoine Chiris in Grasse.

The material was by no means an immediate success. It was simply not understood by many perfumers, and it took almost ten years to introduce the material. During the mid-1960's, many new Nitriles equivalent to "difficult" aldehydes appeared on the perfumery market, and several such Nitriles are now regularly used in perfumes, often under trade names (which is one kind of flattery to the material).

Myristic Nitrile did not become a widely used material, but it did pave the way for other Nitriles by opening the eyes (or the nostrils) of many perfumers to these new chemicals. They have the advantage of being stable in mild alkali and may therefore to a certain degree take the place of aldehydes where these are particularly unstable.

Similar Nitriles exist corresponding to Cinnamic aldehyde, Citral etc.

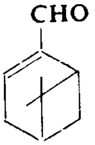
Prod.: from Tridecyl bromide and Potassium cyanide, or:

from Tridecyl magnesium bromide and *Cyanogen chloride* (Grignard).

26-616; B-II-368;
(sample: Antoine Chiris, 1956).

## 2293: MYRTENAL

Benihinal.
A bicyclic monoterpenoid aldehyde of the Pinane group.
The commercial product is *dextro*-Myrtenal.



$C_{10}H_{14}O = 150.22$

Colorless liquid. B.P. 199° C. Sp.Gr. 0.99.

Insoluble in water, soluble in alcohol and oils.

Refreshing, spicy-herbaceous odor of Bayleaf-Cinnamon character. The diffusive warmth is particularly typical (and appreciated).

This aldehyde, rarely found in the price lists from the manufacturers of perfume chemicals, has found good use in perfume compositions, and forms component of many successful perfume bases, etc.

It should have very good opportunity of distribution lately with the revival of the spicy fragrance types. It blends excellently with Oakmoss products, Lavender, Clary Sage, Rosemary, Citrus oils, and with most of the wood notes, Vetiver, Sandalwood etc. or with Opopanax, Patchouli and Styrax for new Oriental notes. Briefly, it is one perfume chemical which is used, but not at all well known. It is rarely seen on the perfumer's shelf, and far too few perfumers have had an opportunity to use it.

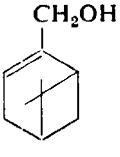
Prod.:

1) by Chromic acid oxidation of Myrtenol (see monograph).
2) by isolation from the higher-than-Cineole fractions in the process of rectifying Eucalyptus oil (E. globulus).

34-806; 67-569; 89-117;

## 2294: MYRTENOL

A bicyclic monoterpenoid alcohol.
**Note**: Do not confuse with "Myrtol", which is a composite of fractions from Myrtle oil.



$C_{10}H_{16}O = 152.24$

Colorless or very pale straw-colored liquid. Sp.Gr. 0.98. B.P. 224° C.

Insoluble in water, soluble in alcohol and oils, not in Propylene glycol.

Warm-herbaceous, slightly woody and discretely "medicinal"-camphoraceous odor of moderate to poor tenacity. The odor is not characteristic of Myrtle leaf or flower, and not typical of Myrtle oil, although this comment is frequently made in perfumery literature.

The fraction section called "Myrtol" consists mainly of the Terpenes from Myrtle oil and is practically free from Myrtenol or Myrtenyl acetate (see next). But "Myrtol" represents the main odor picture of Myrtle oil and has been used as a disinfectant and folks-medicine in the producing areas (Mediterranean).

Myrtenol is an excellent blender-modifier for Lavender, Citrus and Bay type fragrances, for Men's Colognes, etc. and it gives attractive notes to Chypre or Oriental perfumes.

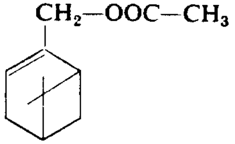
The acetate, which represents the sweetness of the Myrtle oil, is also commercially available and is produced synthetically.

Prod.: – from *alpha-* or *beta-*Pinene

1) by oxidation with Selenium oxide.
2) by chlorination via the acetate to the alcohol. Myrtenal is a by-product in this process.

88-221; 67-569; 163-55;
(sample: Takasago Perfumery Company, Ltd. 1967).

## 2295: MYRTENYL ACETATE



$C_{12}H_{18}O_2 = 194.28$

Colorless mobile liquid.

Insoluble in water, soluble in alcohol and oils.

Pleasant, refreshing, sweet-herbaceous and very slightly spicy-warm odor of moderate tenacity.

This material, only recently made commercially available, offers very interesting effects in Lavender colognes, Citrus complexes, Chypre, Oriental, Fougères, and even in modern variations of the revived Lime fragrance theme.

Its warmth blends excellently into Rosemary, Clary Sage, Lavender, Lavandin, Basil and Estragon, Juniper and Pine needle, etc. It is well supported by Labdanum products, or its sweetness can be increased by the Linalyl esters.

Myrtenyl acetate is usually the largest (single) oxygenated constituent in Myrtle oil (often larger than Myrtenol), except that Cineole (Eucalyptol) is the chief component in certain types of the oil.

However, the title material is now manufactured synthetically.

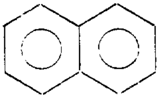
Prod.: from Pinocarveol via its acetate.

Other esters of Myrtenol are known and have been identified in Nature.

90-315; 163-364;

## 2296: NAPHTHALENE

Naphthene.
"Tar camphor".



$C_{10}H_8 = 128.17$

Colorless monoclinic crystals or white crystal scales or leaflets. M.P. 80° C. B.P. 218° C. Sublimes at 45° C. Sp.Gr. 1.16 (solid), but the material floats on boiling water.

Almost insoluble in water, 6% soluble in alcohol, soluble in most oils and in hot alcohol.

Pungent, choking dry-tarry odor of moderate to poor tenacity. The fact that wool, impregnated with Naphthalene vapors will smell of "Naphthalene" for a very long time is based on the presence of impurities of lower vapor pressure in commercial grade Naphthalene.

The vapors are considered hazardous to the human eye (cataract-hazard).

Naphthalene is not used as such in perfume compositions, but it may occur as an impurity, or it may appear as a material of undesirable odor to be overcome by a masking composition. It may also appear as a trace impurity in certain perfume materials.

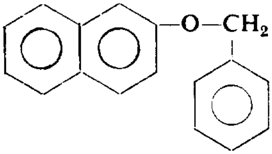
Naphthalene has been used as such for masking of unpleasant odors, but the author finds it questionable whether the Naphthalene odor is really preferred (by the majority of the public) as more acceptable than the odors which it is supposed to overcome.

Prod.: from coal tar. The Naphthalene-rich fractions are pressed and the material purified by sublimation. Certain coal tars contain as much as 10-12% Naphthalene.

26-616; 68-1283; B-V-531;

## 2297: beta-NAPHTHOL BENZYLETHER

Benzyl-*beta*-naphthylether.



$C_{17}H_{14}O = 234.30$

White crystals. M.P. 99° C.

Insoluble in water, soluble in alcohol and oils.

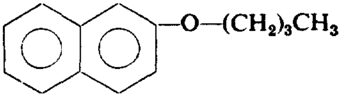
Very mild, sweet-floral-balsamic odor of considerable tenacity.

This material is occasionally used in perfume compositions as a fixative/modifier in Hyacinth, Lilac, Appleblossom and in various floral-fruity or sweet-woody fragrance types, where tenacity and low cost are imperative requirements.

As an odorant, the material has very little to offer, and there are many materials in the same price class and similar tenacity class and even the same odor type as the title material. Most likely, this material will become obsolete and there are many perfume laboratories in which this material never appeared on the shelf.

## 2298: beta-**NAPHTHOL**-n-**BUTYLETHER**

The most common commercial product is the *iso*-Butylether, see next monograph.



$C_{14}H_{16}O = 200.28$

Colorless or white leaflets.

Insoluble in water, soluble in alcohol and oils. The solubility in cold alcohol is rather poor, but always sufficient for compositions.

Intensely sweet and tenacious, fruity-floral-winey odor. In extreme dilution, the fruity notes dominate and resemble (with reasonable imagination) Raspberry. It is characteristic of the *n*-Butylether that it seems more Raspberry-like, while the *iso*-Butylether is generally considered Strawberry-like.

The taste in dilution (below 10 ppm) is sweet and intensely fruity.

This ether has found a little use in perfumery (although the *iso*-Butylether is definitely the most common of the two). It is almost never found in the American price lists from American manufacturers of perfume chemicals, and it is at times absolutely unavailable in the USA. Even the *iso*-Butylether is difficult to obtain. The users may have to manufacture their own material.

The use in flavor compositions is interesting, but restricted. The material is *not* permitted in food flavors in the United States of America.

Prod.: from *beta*-Naphthol and *n*-Butylalcohol (in surplus) by simple esterification with sulfuric acid catalyst/dehydrator. Also from *beta*-Naphtholsodium and *n*-Butylbromide.

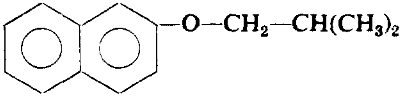
163-226; 5-224;

## 2299: beta-**NAPHTHOL**-iso-**BUTYLETHER**

"Fragarol".

Nerolin-Fragarol.

The *n*-Butylether is known, but the *iso*-Bytylether is the most common commercial item of the two.



$C_{14}H_{16}O = 200.28$

White crystal leaves. M.P. 33° C.
B.P. 307° C.

Practically insoluble in water, soluble in alcohol and oils. The solubility in cold alcohol is rather poor, but generally sufficient for composition.

Sweet and fruity, very tenacious, delicately Neroli-Orangeblossom-floral odor.

The taste in concentrations below 10 ppm is intensely fruity, sweet, of Strawberry-type.

This ether has found some use in perfume compositions, particularly as a fixative and undertone in Citrus colognes, inexpensive Neroli types, etc.

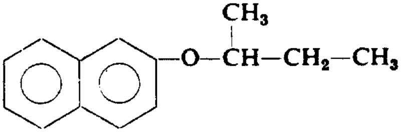
It is also used in flavor compositions – in countries where it is not prohibited – for imitation Strawberry and in various fruit complexes.

The title material is, in the author's opinion, a typical example of a perfume material with excellent virtues, but extremely limited distribution. It is simply unavailable in a number of countries, and very hard to find in the USA. The tendency of the chemical manufacturers to concentrate upon volume chemicals has been very inhibiting to the creative perfumer, although from a profit-making viewpoint it should be understandable that small-volume, low-cost chemicals simply are not interesting. Unfortunately, only a few creative perfume houses have facilities for making their own "small-scale" chemicals, while all the other companies are left without these non-profit-making chemicals. This is how some very simple, old and well-known perfume chemicals end up becoming "captive chemicals" for the house that really wants them.

Prod.: by simple etherification of *beta*-Naphthol with a surplus of *iso*-Butanol under reflux in the presence of sulfuric acid. It has also been prepared from the sodium salt of *beta*-Naphthol with *iso*-Butylbromide.

5-224; 17-71; 156-294; 163-55; 163-226;

## **2300:** beta-**NAPHTHOL**-secondary-**BUTYLETHER**



$C_{14}H_{16}O = 200.28$

Colorless or white shiny leaflets or scale-like crystals. M.P. 34° C. B.P. 298° C.

Insoluble in water, poorly soluble in cold alcohol (about 6%), soluble in hot alcohol and most perfume oils.

Delicate and sweet, very tenacious floral-fruity odor. Less fruity than the *iso*-Butylether, more Neroli-like in dilution.

This ether, practically unavailable on the market, but occasionally manufactured by the user, has been suggested for use in soap perfumes because of its low cost, great stability and excellent odor value.

It seems that the names Yara-Yara or *beta*-Naphthol - - - have impregnated the perfumers' minds with an association of "cheap" odors. But in the proper creative hands, these materials can do small wonders, and this is just one more of the encouraging phases of creative perfumery – the unconventional use of raw materials.

Most of the *beta*-Naphthol ethers have, when sufficiently purified, quite attractive odors in the proper dilution. And they are excellent fixatives in soap perfumes.

The title material would do very well in new versions of "Cashmere bouquet" type fragrances, Oriental bouquets, and it has very interesting effects in sophisticated Pine needle fragrances.

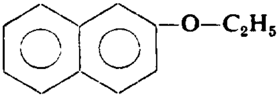
Prod.:

1) from *beta*-Naphthol and *secondary*-Butylalcohol in the presence of sulfuric acid, or:
2) from *beta*-Naphtholsodium and *secondary*-Butylbromide.

5-224; 163-226;

## **2301:** beta-**NAPHTHOL ETHYLETHER**

"Bromelia".
Nerolin Bromelia.
*2*-Ethoxynaphthalene.
Ethyl-*beta*-naphthylether.
Nerolin II.
Ethyl-*2*-naphthylether.



$C_{12}H_{12}O = 172.23$

White, shiny crystals or leaflets. M.P. 37° C. B.P. 282° C. Sp.Gr. 1.06 (liquid).

Insoluble in water; soluble in alcohol and oils, poorly soluble in Propylene glycol. The solubility in alcohol is much better than that of the -methylether (Yara-Yara).

This ether is one of the two "conventional Nerolins" in perfumery use. Its soft, floral and very tenacious Neroli-note is appreciated by most perfumers who have used it, while it may take some convincing to overcome the resistance of "first-time users", because of the apparent harshness of the pure chemical. It is more powerful than most people think, and its value is mainly "odor-value" – good odor effect for a very modest cost.

As a sweetener and floralizer, it is used frequently with Methylnaphthyl ketone, Methylanthranilate, Petitgrain oil, etc. and it blends very well with Linalool and esters, Terpineol and esters, *iso*-Butylphenylacetate, traces of Undecanolide, etc. Interesting effects are achieved by proper fixative balancing with equally high boiling materials, e.g. Amylcinnamic aldehyde, etc. The material is stable in soap and very resistant to heat. Modern household products include several problems where heat-resistant fragrances are needed.

The title ether is used in trace amounts in flavor compositions, mainly in fruit complexes, berry compositions, Honey and Nut imitations, etc. In extreme dilution, the flavor is mainly fruity, sweet and Grape-Strawberry-like. The *iso*-Butylether is far superior as a Strawberry material, but it is *not* permitted in food flavors in the USA. Concentrations of the ethylether will be about 0.1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2768.

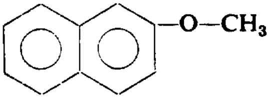
Prod.:

1) from *beta*-Naphthol and Ethylalcohol with sulfuric acid.
2) from *beta*-Naphtholsodium in weak aqueous alkali with Diethylsulfate.
3) from *beta*-Naphtholsodium and Ethylbromide.

5-223; 26-546; 68-1309; 95-119; 96-105; 106-278; 163-55; 163-226; B-VI-641;

## 2302: beta-**NAPHTHOL METHYLETHER**

"Yara-Yara".
Nerolin Yara-Yara.
Nerolin I.
*2*-Methoxynaphthalene.
Methyl-*beta*-naphthylether.



$C_{11}H_{10}O = 158.20$

White shiny crystal leaves. M.P. 73° C. B.P. 274° C.

Sublimes when heated. Almost insoluble in water, 4% soluble in cold alcohol, somewhat better in hot alcohol, miscible with most perfume oils.

The odor of highly purified material is intensely sweet, Orangeblossom-Acacia-like, very tenacious, but many commercial grades are poorly refined and display rather harsh notes, an odor description generally used for this material. It is, indeed, more agressive than the Ethyl-ether, but at the reasonable use-level, the odor is free from harshness, displays only power and intense sweetness. Perhaps the fact that the floral note is somewhat "off-natural" contributes to the discouraging odor description.

This ether is used extensively in low-cost fragrances for household products, soaps, detergents (but rarely in dishwashing detergents), and particularly in products where heat-and-alkali-stability are required. It is also used as masking odor for acrylic or other "plastic" odors, synthetic rubbers, etc., which requires good retentiveness.

A very inexpensive, non-purified grade is available for industrial masking purposes, and it offers powerful odor and good fixation. There is a considerable difference in price between the crude and the refined grades. The crude reaction product can be melted and/or extracted with Tetrachloromethane directly from the reaction vessel. This product is brownish, dark amber-colored or pale purple colored, usually in lumps of crystalline structure. Recrystallization or sublimation or vacuum-distillation via heated condenser produces the white refined product.

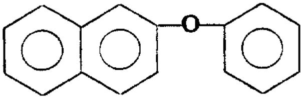
Prod.: from *beta*-Naphtholsodium with Dimethylsulfate in weak aqueous alkali.

Also from *beta*-Naphthol and a surplus of Methanol under reflux with sulfuric acid catalyst.

5-223; 26-608; 61-75; 68-1309; 95-119; 96-105; 106-349; 156-293; 163-55; 163-226; B-VI-640;

## 2303: beta-NAPHTHOL PHENYLETHER

Phenolnaphthylether.
"Phenylnaphthyloxide".



$C_{16}H_{12}O = 220.27$

White crystals. M.P. 46° C. B.P. 252° C.

Practically insoluble in water, soluble in alcohol and oils.

Delicately sweet and tenacious, floral-balsamic odor of Neroli-Hyacinth-Narcisse type. There are notes in this complex of a pleasant fruity character, reminiscent of Apricot. This is interesting because Neroli oil is an old "trick" in imitation Apricot flavor, but not all Neroli-perfume materials are suitable for Apricot.

The title ether is very rarely seen in price lists, but it may be prepared by the user himself in a few cases. It is stable in soap and very resistant to heat.

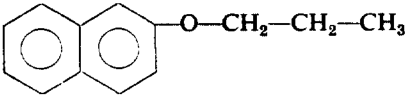
Prod.:
1) from Phenol and *beta*-Naphthol by heating with Aluminum chloride to 350° C.
2) same – using Zinc chloride.

The yields are reported to be very poor.

68-1309; 96-105; 163-226; 163-365;

## 2304: beta-NAPHTHOL PROPYLETHER

*n*-Propyl-*beta*-naphthylether.
*2*-Propoxy naphthalene.



$C_{13}H_{14}O = 186.26$

Colorless needlelike crystals. M.P. 40° C. B.P. 300° C.

Insoluble in water, soluble (about 8%) in cold alcohol, better in hot alcohol and in most perfume oils.

Very sweet and delicate fruity-floral odor of excellent tenacity. The floral notes are discretely neroli-like, while the fruity notes have a remote resemblance to Strawberry.

This ether, very rarely offered commercially, has found a little use in perfume compositions for its persistant odor and intense sweetness. It can be produced at a very attractive cost, and it is stable in soaps or against heat. With Hydroquinone dimethylether in Hyacinth compositions, or with Ethyl methyl phenyl glycidate in Rose variations, it may give very interesting results.

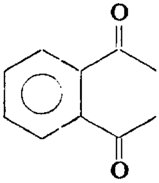
Its character is overall fresher than that of the Methyl and Ethyl ethers, while it is less fruity than the *iso*-Butylether.

Prod.: from *n*-Propylalcohol (in surplus) with *beta*-Naphthol and sulfuric acid, by refluxing for 6 hours.

163-226; (private experiments);

## 2305: alpha-1,4-NAPHTHOQUINE

*1,4*-Dihydro-*1,4*-diketonaphthalene.



$C_{10}H_6O_2 = 158.16$

Yellow crystals. M.P. 126° C. Sublimes before melting. Sp.Gr. 1.42 (liquefied).

Intensely sweet, but unpleasant, almost choking odor. In high concentration it may remind the observer of Halogen-odor, and a great variety of phrases are used for description of its odor.

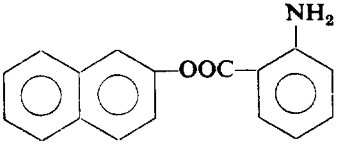
The material has been used for masking of unpleasant industrial chemical odors, but the author believes that this practice is obsolete.

Prod.: by chromic acid oxidation of *1,4*-Amino-naphthol.

26-618; 31-84; 100-705; 160-1116; B-VII-724;

## **2306:** beta-**NAPHTHYL ANTHRANILATE**

*2*-Naphthyl-*ortho*-aminobenzoate.



$C_{17}H_{13}NO_2 = 263.30$

Pale straw-colored or almost colorless liquid, solidifying in the cold. B.P. 340° C. Sp.Gr. 1.03.

This ester is the kind of perfume material which is more talked about in literature than used in the laboratory.

Undoubtedly, the idea of making an ester from Naphthol which had a record of many successful Orange-blossom type derivatives, with Methylanthranilate, long since established as an Orangeblossom chemical, seems almost too obvious.

The result, often very poorly purified, is a material with a rather harsh Orangeblossom odor. Much more dry than Methylanthranilate, and not nearly as versatile.

The author believes that this material may as well disappear from the perfume laboratory shelves. Very few perfumers will miss it.

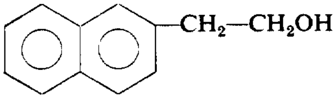
It is, curiously enough, permitted in food flavors, where it is used at the concentration of up to 20 ppm in the finished product to introduce a Grape-like note (fixative) or as a fixative in fruit complexes.

G.R.A.S. F.E.M.A. No.2767.

Prod.: from Isatoic anhydride and *beta*-Naphthol. Older methods produced very impure material, a type still in use.

34-1022; 103-165; 163-55; 163-227;

## **2307:** beta-**NAPHTHYL ETHYLALCOHOL**



$C_{12}H_{12}O = 172.23$

Colorless or white crystals or crystalline powder. M.P. 62° C. B.P. 288° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, woody-camphoraceous, musty odor of considerable tenacity.

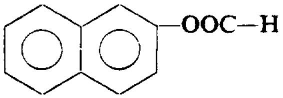
Although often mentioned in perfume literature, this material seems rather uninteresting. Derivatives of the completely hydrogenated Naphthol (Decalinol) include many interesting perfume chemicals, but the title material lacks character. It is not an Ambregris chemical, and it is not a clean woody type. It has tenacity and it may give a lift to soap perfumes of the woody-Patchouli-like type. The author believes that this material can be considered almost obsolete as a fragrance chemical.

Prod.: from *1*-Naphthyl magnesium bromide plus Ethylene oxide.

68-1326;

## **2308:** beta-**NAPHTHYL FORMATE**

*2*-Naphthyl methanoate.



$C_{11}H_8O_2 = 172.19$

White crystalline powder.

Insoluble in water, soluble in alcohol, miscible with oils.

Peculiar, dry-green, musty-medicinal odor with warm-herbaceous character. Good tenacity.

This ester has been suggested for use in

perfume compositions for its very peculiar odor which, to some observers, resembles that of Blackcurrant buds.

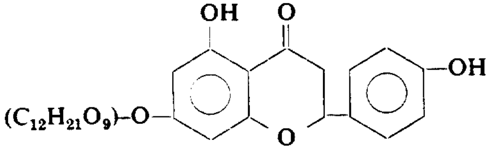
The occurrence in the Plant Kingdom of Naphthalene derivatives was for a long time considered to be out of the question. However, *beta*-Naphthol has been identified in the volatile oil of Blackcurrant buds (Dr. Georges Igolen, 1937) and it seems conceivable that its mission is partly that of being an antioxidant to protect the natural aldehydes in the plant (oil).

It is furthermore interesting to notice that the American authorities do not recognize more than one Naphthylether (Ethyl-) and one ester (-anthranilate) for use in food flavors.

The artificial reconstruction of Blackcurrant flavor has always been considered by flavorists as one of the most difficult tasks, and the components so far identified show that the key flavor ingredients in Blackcurrant belong to very unusual chemical groups.

## 2309: NARINGIN

A 7-Rhamnoglucoside of *5:7:4'*-trihydroxyflavanone.



Carbohydrate-
radicle =
2 × Rhamnose.

$C_{27}H_{32}O_{14}$, $8H_2O$ = 724.68
(580.55 + 144.13)

White amorphous or microcrystalline powder. M.P. 83° C.

Soluble in water and diluted alcohol, not soluble in oil.

This material has been identified, isolated and commercially extracted from the Grapefruit, mainly from the non-edible white part of the inner peel (the "albedo" section).

It is one of the bitter principles in the peel and other parts of the fruit. The material is virtually odorless and it has a clean, bitter taste, although not excessively powerful.

It has been suggested as a replacement for Quinine in bitter tonics, "Quinine water", "Grape-tonic" (a Grapefruit drink), etc. in countries (e.g. Japan) where the use of Quinine in soft drinks is either prohibited or restricted.

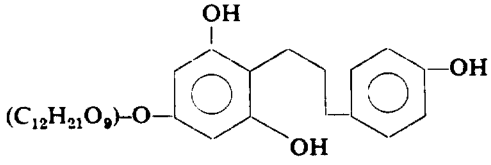
Part of the subject molecule is closely related to the Coumarins and to *para*-Hydroxycinnamic acid. Other Coumarin derivatives are found in great variety in the Citrus fruits.

Naringin is listed as G.R.A.S. in the U.S. Federal Register, and it has found extensive use as a natural flavor extractive.

Prod.:
1) by extraction from Grapefruit peel.
2) synthetic (Japanese patent).

66-1209; 66-1282; 69-958; 158-128;
(Sample: Exchange Citrus fruit growers, California, USA)
(see also following monograph).

## 2310: NARINGIN DIHYDROCHALCONE



Carbohydrate-
radicle.

$C_{27}H_{34}O_{14}$ = 582.57

White powder.

Practically odorless. Pleasant, sweet taste in water. Estimated sweetness is 100 times that of cane sugar.

This material, only recently developed, has been suggested as a sweetener in future food products, particularly dietetic foods, low-calorie foods, juices, beverages, etc.

A dihydrochalcone from a related natural material, extracted from the Seville Orange (see Neohesperidin dihydrochalcone) appears to be much sweeter than the subject material.

However, the "medium-strength" sweeteners may have a much better chance of acceptability among the consumers than the very powerful sweeteners. For several reasons:

Sweet taste reception varies considerably according to the subject (person). Very powerful sweeteners tend to leave a bitter or unpleasant aftertaste in the mouth and on the lips (an apparent counter-action).

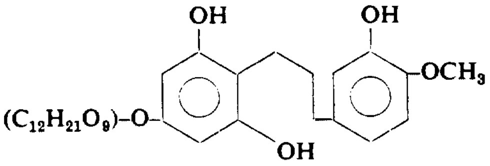
The title material has *not* yet (Sept. 1968) been included in the authoritative or official lists as approved for use in food.

Prod.: from Grapefruit-naringin via its Chalcone, followed by catalytic reduction to the title material.

158-128;
See also: Chemical & Engineering News, Oct. 17, 1966, page 114.

## 2311: NEOHESPERIDIN DIHYDROCHALCONE

The hydrogenated chalcone of the *7-beta*-Rutinoside of *5:7:3'*-Trihydroxy-*4'*-methoxyflavanone.



Carbohydrate-
radicle (Rutinose).

$C_{28}H_{36}O_{15} = 612.60$

White powder. Soluble in water and diluted alcohol. Practically insoluble in oils.

Virtually odorless. Intensely sweet taste in water. Estimated sweetening strength is 2400 times that of cane sugar.

This material was developed shortly after the discovery that Naringin dihydrochalcone was sweet tasting (while Naringin itself is bitter).

It has been suggested as a possible sweetener in future foods, particularly dietetic foods, low-calorie candy, soft drinks, juices, etc.

At the time of editing this monograph, the material has *not* yet been officially approved for use in foods in the USA (Sept. 1968).

Prod.: from Neohesperidin (an isomer of Hesperidin), derived from the peel of the Seville Orange (the albedo part specifically).

69-958;
See also: Chemical & Engineering News, Oct. 17, 1966, page 114.

## 2312: NEO-IRONES

A summary of naturally occurring and olfactorily interesting Neo-irones.

Of the ten known isomers of Irone, the following four have been identified in Nature (other than *alpha*-Irone) and they have generally been described as interesting from a perfumery point of view:

NEO-*alpha*-IRONE:
*cis-2,6-trans-2'-2"-alpha*-Irone.

Colorless liquid, Sp.Gr. 0.93. Odor very similar to that of *alpha*-Irone.

Produced from Orris oil.
89-404; 163-208;

NEO-*iso-alpha*-IRONE:
*trans-2,6-trans-2'-2"-alpha*-Irone.

Colorless liquid. Sp.Gr. 0.93. Good Violet character.

Produced from synthetic *dl*-Neo-*iso-alpha*-Irone via the Menthylaminocarbonate.
89-405; 163-208; 163-365;

NEO-*beta*-IRONE:
*trans-2'-2"-beta*-Irone.

Colorless liquid. Sp.Gr. 0.95. More woody and dry than *alpha*-Irone.
89-405; 159-449; 163-227;

NEO-*gamma*-IRONE:
*cis-2,6-trans-2′-2″-gamma*-Irone.

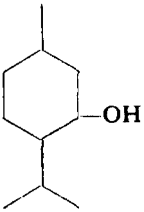
Colorless liquid. Sp.Gr. 0.94. Very poor stability. More woody and green than *alpha*-Irone.

Produced from Orris oil (or rhizome) by distillation under *neutral* conditions. Normal conditions are *acid*, rarely alkaline.
89-405;

See also monographs: *alpha*-Irone,
*beta*-Irone and
*gamma*-Irone.

## 2313: dextro-**NEOMENTHOL**

*3-para*-Menthanol.
*1*-Methyl-*4-iso*-propylcyclohexan-*3*-ol.
*trans-1*-Methyl-*cis-4-iso*-propylcyclohexanol.



$C_{10}H_{20}O = 156.27$

White or colorless crystals. M.P. 52° C. but may remain supercooled as a colorless oily liquid. Sp.Gr. 0.90. B.P. 212° C.

Very slightly soluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol, moderately soluble in mineral oil.

Refreshing Menthol type odor, but not quite as sweet as Menthol. The taste is similar to that of Menthol at very low concentrations, but at concentrations higher than 5 ppm, there is more cooling effect from *laevo*-Menthol than from the title material.

This material is used as an "extender" for Menthol and Peppermint oils. Although it has been identified in certain types of Peppermint oil, this alcohol is not very popular as a flavor item. At concentrations normally used, the effect is not only less cooling, but the title alcohol carries with it a "musty" or "flat" odor which tends to detract from a Peppermint or Menthol aroma-picture, rather than lifting it.

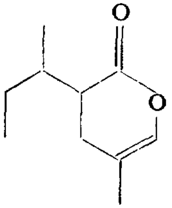
This alcohol is not used very extensively in perfume compositions. *dl*-Menthol is usually preferred for this type of "lift" unless the superior *laevo*-Menthol is used.

Prod.: synthetic from *dl*-Menthone by Meerwein-Ponndorf-Verley reduction.

G.R.A.S. F.E.M.A. No.2666.

65-226; 88-13; 88-36; 163-46; 163-365;
B-VI-28;
See also: *dextro*-Menthol.

## 2314: **NEPETALACTONE**



$C_{10}H_{14}O_2 = 166.22$

Pale yellowish oil. B.P. near 300° C.
Sp.Gr. 1.07.

Practically insoluble in water, soluble in alcohol and oils.

Warm-spicy and very tenacious odor with an almost choking sweetness often classified as "nauseating".

This lactone is mentioned briefly in this work because it has found extensive use as a catlure. It may therefore be of interest to those who study the odor preferences of certain animals. The perfumer is occasionally faced with the problem of developing a fragrance (or an "odor") to attract dogs, or to repel dogs, to repel rabbits, etc. etc. and it can be quite a problem since only very meager information can be found in literature.

Prod.:

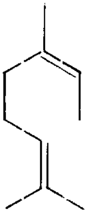
1) by isolation from American catnip oil (about 45% lactone).
2) synthetic, from Ethyl-*3*-methyl-*2*-oxocyclopentane carboxylate with Bromo butyne.

90-661; 100-714;

## 2315: NEROL

*2-cis-3,7*-Dimethyl-*2,6*-octadien-*1*-ol.
"Lorena" (Firmenich).
Nerosol.
Nerolol.
Nerogenol.
Allerol.
Neraniol.
Nerodol.
- and many other trade names.

Most of the above trade names represent mixtures of Nerol with variable amounts of Geraniol (the *trans*-isomer).



$C_{10}H_{18}O = 154.25$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 227° C.

Very slight soluble in water, soluble in alcohol and oils.

Sweet rosy, refreshing and "wet" seashore odor of moderate tenacity. Dry notes vary with purity of material. A very pure Nerol will normally have more emphasis on the "fresh seashore" odor and less of the rosy notes, while products with high Geraniol content conceal their "maritime" notes in favor of the deep-rosy tones.

Sweet and rosy-fruity taste; in concentrations below 10 ppm the fruitiness dominates and become more Raspberry-like, less rosy.

This alcohol is widely and frequently used in perfumery, but not nearly in the volumes of Geraniol and Citronellol. It lends a freshness to a rose base which cannot be obtained with the two other alcohols. But it also finds use in a variety of sweet-floral fragrance types, Mimosa, Magnolia, Lilac, Neroli, Alpine Violet, Jasmin, etc. or in Citrus colognes, Muguet, Orchid, etc. its effect is perceptible often at one or two percent in the composition.

Nerol is also used in flavor compositions for its Raspberry-Strawberry effect, in fruit complexes (its tenacity is superior to that of the conventional items) and in Honey bases. A special use is that in imitation terpeneless Lemon oil.

Concentrations in the finished product vary from 1 to 20 ppm.

Prod.:

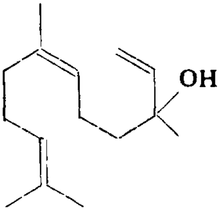
1) by reduction of Citral via the Meerwein-Pondorf-Verley type reaction, resulting in a Geraniol-Nerol mixture with 60-70% Nerol.
2) from Pinene via Myrcene to a Geraniol/Nerol mixture from which the Nerol is isolated via Calciumchloride removal of Geraniol or by careful fractionated distillation. $CaCl_2$ does *not* form an adduct with Nerol, only with Geraniol.

G.R.A.S. F.E.M.A. No.2770.

87-568; 100-715; 106-276; 156-166; 160-1122; 163-56;

## 2316: NEROLIDOL

*3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-ol.
Methyl vinyl homogeranyl carbinol.
"Peruviol" (old, abandoned name, see also Benzylcinnamate).
The commercial, synthetic product consists mainly of the *cis*-isomer.



$C_{15}H_{26}O = 222.37$

Colorless or very pale straw-colored oily liquid. Sp.Gr. 0.88. B.P. 276° C:

Very slightly soluble in water, soluble in alcohol and oils. The material shows some tendency of resinification (polymerization) upon exposure to air (poor storage conditions).

Mild and delicately woody-floral, slightly green odor with remote resemblance to Apple and Lily. The tenacity is excellent but shows variations according to origin of material.

The title material is almost typical of modern chemistry in perfume raw materials: In 1950, it was still a rare and very expensive material (U.S. $ 150.00 per kilo) and only used in the most exquisite floral or fine woody perfumes. Ten years later, a new synthesis and a freely available natural oil brought the price down to $ 40 or 30 per kilo, and today, it is available as a purely synthetic material for about $ 15.00 per kilo, while an essential oil, containing 80% Nerolidol, is occasionally available at less than half that price.

Yet, it seems as if there are still perfumers who think of Nerolidol as an "expensive" raw material, and subconsciously avoid the use of it. It is actually an extremely useful chemical, not only because of its delicate and very versatile notes, but also because of its fixative value and blending properties.

The title alcohol is an excellent "fond" in Sweet Pea, Muguet, Honeysuckle, Peony, etc., and a fine companion to Sandalwood, Oakmoss, Perubalsam, Tolubalsam, Clary Sage products, Ylang-Ylang, etc.

It finds limited use in flavor compositions as a trace component in imitation Honey, Apple, Rose, and in Citrus complexes, Berry flavors and fruit blends. The concentration used is normally only 1 to 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2772.

Prod.:

1) from Geranylacetone plus Acetylene, followed by reduction of the acetylenic linkage (Hoffmann-laRoche process).
2) by isolation from Cabreuva oil or other essential oils.

31-20; 88-239; 100-715; 104-108; 104-409; 104-463; 106-277; 156-375; 163-56; 163-227;

## 2317: NEROLIDYL ACETATE

*3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl acetate.

$C_{15}H_{25}—OOC—CH_3$

$C_{17}H_{28}O_2 = 264.41$

For structure – see Nerolidol.

Colorless liquid. Sp.Gr. 0.91. B.P. 280° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-woody, tenacious and mildly green-refreshing odor.

This material is probably one of the least interesting of the Nerolidyl esters, in spite of the fact that it is the only one so far identified in Nature (Clary Sage oil and Neroli oil).

It may find some use as a modifier for the alcohol in Muguet bases or other light florals, or as a blender for Sandalwood odor in woody Oriental bouquets, but it does not contribute much odor or character.

Prod.: (several methods), e.g. by low-temperature acetylation of Nerolidol. Also via Acetylation of Dehydronerolidol, followed by hydrogenation.

163-365; 90-323;
See also: Hoffmann-laRoche data.

## 2318: NEROLIDYL-iso-BUTYRATE

*3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl-*iso*-butyrate.
For structure – see Nerolidol.

$C_{15}H_{25}—OOC—CH(CH_3)_2$

$C_{19}H_{32}O_2 = 292.47$

Colorless oily liquid. Sp.Gr. 0.89.

Practically insoluble in water, soluble in alcohol and oils.

Very sweet, fruity-woody, Bergamot-and-Pear-like, but delicate and very tenacious odor.

This is one of the more interesting esters of Nerolidol with great versatility and interesting possibilities. At the present price of Nerolidol and its esters, this material can be used in almost any type of perfume with little or no cost restriction.

As part of the fixative base in Bergamot type colognes, as fixative in Men's Lime fragrances, as companion to Oakmoss in novel type Fougères, and as blender for the Methylionones, it has almost endless possibilities. In Neroli bases or as an undertone in Magnolia and Peony, in lipstick perfumes with Ethyl methyl phenyl glycidate, etc. it gives the perfumer a wealth of new ideas.

It could undoubtedly find use in flavor compositions if it were permitted in food flavors. Its Bergamot-Pear-Lemon-Raspberry complex could be utilized in an interesting way.

Prod.: from Nerolidol by low-temperature esterification with *iso*-Butyric acid (or anhydride), e.g. by azeotropic esterification.

Also via Dehydronerolidol (see Nerolidol).

163-365;
See also: Hoffmann-laRoche data (catalogue).

## 2319: NEROLIDYL FORMATE

*3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl formate.
For structure – see Nerolidol.

$C_{15}H_{25}—OOC—H$

$C_{16}H_{26}O_2 = 250.38$

Colorless liquid. Sp.Gr. 0.92.

Practically insoluble in water, soluble in alcohol and oils.

Delicately woody, rather dry, but refined and discrete odor of moderate to good tenacity. It has a touch of floral note which, combined with the woody and green traces make this material almost "confined" to Muguet.

This ester is of little interest to the perfumer, except that it can supply an interesting variation of the Muguet theme, and it can add attractive notes to a woody-ambre-like composition. It blends very well with Galbanum and Styrax, or with certain of the higher carbinols.

Prod.: by cold formylation of Nerolidol.

163-365;
See also: Hoffmann-laRoche data (catalogue).

## 2320: NEROLIDYL PROPIONATE

*3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl propionate.
For structure – see Nerolidol.

$C_{15}H_{25}—OOC—C_2H_5$

$C_{18}H_{30}O_2 = 278.44$

Colorless liquid. Sp.Gr. 0.91.

Practically insoluble in water, soluble in alcohol and oils.

Fresh, but rather dry, delicately woody, remotely Pear-like odor of pleasant softness and good tenacity.

This ester is almost as uninteresting as the acetate. It may find some use in perfume compositions for its peculiar green-fruity-woody effect which blends excellently with Cyclamen aldehyde, etc.

It is commercially available, but very rarely found on the perfumer's shelf, except as a sample bottle.

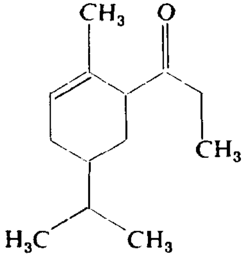
Prod.: by azeotropic type esterification of Nerolidol with Propionic acid.

Or via Dehydronerolidol – see Nerolidol process.

163-365;
See also: Hoffmann-laRoche catalogue.

## 2321: NERONE

The title name is Givaudan Corporation's trade name for:
*1*-(*para*-Menthen-*6*-yl)-*1*-propanone.
Menthenyl ketone. (The commercial material is a mixture of *cis*- and *trans*-isomers).
The *cis*-isomer is olfactorily preferred but not separately available.



Main component (*cis*-Nerone).

$C_{13}H_{22}O = 194.32$

Colorless or very pale straw-colored oily liquid. Sp.Gr. 0.92.

Almost insoluble in water, soluble in alcohol and oils.

Warm and bitter-sweet, green-floral, woody-leafy odor of moderate tenacity. The undertones are warm, almost Honey-like.

The material shows tendency of acquiring an acid topnote after long-time or improper storing, quite typical of chemicals containing an acetyl sidechain (or propionyl-).

The odor is generally described as Petitgrain-like, and there is no other commercially available chemical of a more Petitgrain-like character.

The title ketone finds considerable use in perfume compositions for soap, detergent and cosmetic preparations where its stability in finished compounds is greatly appreciated.

For novel and sophisticated "Mimosa" or "Nectar" fragrance bases, it offers unique notes, unobtainable with any other chemical. As part of the warm notes in Chypre or modern Citrus colognes, New Mown Hay and Oriental bases, it gives the perfumer a wide variety of applications.

Although this ketone can be considered as a derivative of an isomer of Dihydrocarveol, it was for a long time regarded as an "unnatural" perfume chemical. It is very conceivable, however, that Nerone exists in natural oils.

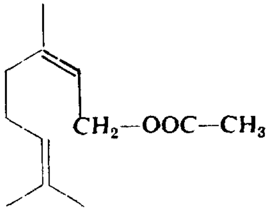
Prod.: Givaudan pat. 3,007,967 of 7th Nov. 1961. (USA).

From *1*-*para*-Menthene with Propionic anhydride at 30° C in presence of Zinc chloride.
106-279; 156-376; 163-365; 159-476;

Givaudan data sheet of Sept. 1959.

## 2322: NERYL ACETATE

*2-cis-3,7*-Dimethyl-*2,6*-octadien-*1*-yl acetate.



$C_{12}H_{20}O_2 = 196.29$

Colorless oily liquid. Sp.Gr. 0.91.
B.P. 231° C.

Very slightly soluble in water, soluble in alcohol and oils, somewhat soluble in Propylene glycol.

Very sweet, fruity-floral odor of Raspberry-Rose character, refreshing and moderately tenacious.

Very sweet, deep-fruity taste in concentrations below 10 ppm, Raspberry-Citrus-like. Higher concentrations tend to appear "perfumey".

This ester finds use in perfume compositions, when cost allows for it, for Neroli, Jasmin, floral and fruity fragrance types. It costs several times more than Geranyl acetate, but has much more sweet and fruity power. Unfortunately, there are poorer grades of Nerylacetate on the market containing significant amounts of Geranylacetate which conceals the true olfactory effect of the title ester.

The material finds some use in flavor compositions, mainly in Citrus, Neroli, Honey, Raspberry, fruit complexes, etc. where sweetness is essential with warm-fruity notes.

The concentration in the finished product will normally be about 1 to 15 ppm.

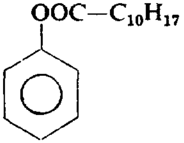
Prod.: (several methods) e.g. as a by-product in the manufacture of Geranylacetate from Myrcene by Hydrobromination and esterification.

G.R.A.S. F.E.M.A. No.2773.

4-103; 33-503; 86-103; 90-266; 106-280; 104-292; 156-272; 36-174; 163-56; 163-227;

## 2323: NERYL BENZOATE

Structure and chemical name – see: Neryl acetate.



$C_{17}H_{22}O_2 = 258.36$

Colorless viscous liquid. Sp.Gr. 0.97.
B.P. 325° C.

Insoluble in water, soluble in alcohol and oils.

Very mild, floral-balsamic and slightly "metallic"-fresh odor, sometimes described as "green". Excellent tenacity.

This ester could find use in perfume compositions such as heavy floral fragrances, exotic-balsamic, woody florals, Ylang-Ylang, etc. However, since its effect is quite similar to that of Geranyl benzoate which is much less expensive, there is not much demand for the title ester. As a fixative, it is generally too costly, and its odor contribution to a fragrance does not justify its relatively high price.

Prod.: from Benzyl chloride and Nerol, using a Pyridine type catalyst.

36-174; 163-56;

## 2324: NERYL BUTYRATE

Neryl-*n*-butyrate.

$C_{10}H_{17}—OOC—CH_2—CH_2—CH_3$

$C_{14}H_{24}O_2 = 224.35$

Structure and chemical name – see: Neryl acetate.

Colorless liquid. Sp.Gr. 0.89. B.P. 240° C.

Almost insoluble in water, soluble in alcohol and oils.

Delicate, leafy-floral, fruity Orange-like and very sweet odor of moderate tenacity.

Sweet-fruity, heavy "fruitpreserve"-like taste in concentrations around 10 ppm.

This ester finds a little use in perfume compositions as a modifier in Lilac, Lily, Neroli, Rose and other florals. Its discretely animal character makes it particularly suitable for Rose and Lilac, while its leafy-fruity notes blend well with Citrus and Neroli notes.

The ester is also used in flavor compositions. The same discretely animal-heavy notes are useful in Cocoa, Chocolate and many Berry-types, in fruit complexes and Citrus flavors. The concentration is normally about 5 to 25 ppm in the finished product.

Prod.: by azeotropic esterification of Nerol with Butyric acid (or by ordinary esterification with Butyric anhydride).

G.R.A.S. F.E.M.A. No.2774.

33-734; 36-175; 163-56; 163-227;

## 2325: NERYL-iso-BUTYRATE

$C_{10}H_{17}$—OOC—$CH(CH_3)_2$

$C_{14}H_{24}O_2 = 224.35$

Structure and chemical name – see: Neryl acetate.

Colorless liquid. Sp.Gr. 0.94. B.P. 232° C.

Practically insoluble in water, soluble in alcohol and oils.

Very delicate, refreshingly floral-sweet and warm odor of moderate to good tenacity. The ester seems to be generally preferred for stability over the *n*-Butylester, while the odor difference between the two is conspicuous enough to classify them as two separate fragrance materials, some perfumers preferring one odor, others the second.

This ester finds limited use in fragrance compositions where it may lend richness ("body") and deep sweetness to Citrus or light floral bases, Rose and novelty types. As a variant in Honeysuckle, Gardenia, etc. it is also of some interest.

The subject material is used in flavor compositions for sweetness in Citrus flavors and fruit complexes. It seems to be more difficult to discriminate between the *flavors* of the *iso*-Butyrate and the *n*-Butyrate than it is for the *odor* of the two. The title ester is normally used in mere traces in the finished product.

G.R.A.S. F.E.M.A. No.2775.

Prod.: by azeotropic esterification of Nerol with *iso*-Butyric acid or by ordinary esterification with *iso*-Butyric anhydride.

33-734; 36-175; 163-56;

## 2326: NERYL CAPROATE

Neryl hexylate.
Neryl hexanoate.
Neryl hexoate.
For structure and full chemical name, see: Neryl acetate.

$C_{10}H_{17}$—OOC—$(CH_2)_4CH_3$

$C_{16}H_{28}O_2 = 252.40$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Refreshing, sweet-rosy or fruity-herbaceous odor with emphasis on the fruity (fruit-preserve)-notes, and less floral than the lower esters of Nerol.

This ester is very rarely offered commercially, but has been suggested for use in perfume compositions, where it blends very well with items such as Clary Sage and Lavender, giving depth and background, tenacity and sweetness.

Prod.: by azeotropic esterification of Nerol with Caproic acid. (*n*-Hexanoic acid).

163-56; 163-227;

## 2327: NERYL FORMATE

$C_{10}H_{17}—OOC—H$

$C_{11}H_{18}O_2 = 182.27$

For structure and full chemical name – see: Neryl acetate.

Colorless liquid. Sp.Gr. 0.92. B.P. 225° C.

Almost insoluble in water, soluble in alcohol and oils.

Refreshing herbaceous-green and floral, delicately rosy (like hedgerose) odor of moderate tenacity.

Sweet and tart-fruity, rich flavor in concentrations near 10 ppm.

This ester is used occasionally in perfume compositions for its delicately green-leafy, floral effect, equally suitable for Rose and for Violet. With Clary Sage and Rose materials it may create very attractive tearose notes.

The ester is also used in flavor compositions, mainly in imitation Apricot, Peach, Apple, Pineapple and in fruit and Citrus complexes at concentrations equal to 5 to 25 ppm in the finished product.

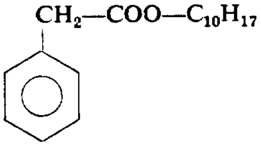
Prod.: by cold formylation of Nerol.

G.R.A.S. F.E.M.A. No.2776.

36-174; 163-56; 163-227;

## 2328: NERYL PHENYLACETATE

Neryl-*alpha*-toluate.



$C_6H_5—CH_2—COO—C_{10}H_{17}$

$C_{18}H_{24}O_2 = 272.39$

For full structure and chemical name – see: Neryl acetate.

Colorless viscous liquid. Sp.Gr. 0.95.
B.P. 327° C.

Practically insoluble in water, soluble in alcohol and oils.

Deep-sweet, very rich, but mild-rosy-honey-like, floral odor of considerable tenacity. The undertones may be ruined by a surplus of Phenylacetic acid if such is present.

This ester, rarely offered commercially, is occasionally used in perfume formulations where it may introduce heavy-sweet undertones and richness, fixative value and discretely honey-like notes. If it were not for cost problems, the ester could be used at very high concentrations, e.g. 10-25% in a composition, but it is often replaced by Geranyl phenylacetate for such purposes. For finer perfumery, however, it may be used quite freely for all types of exotic and heavy florals, etc.

Prod.: by azeotropic esterification of Nerol with Phenylacetic acid, or from Nerol and Phenylacetyl chloride.

7-298; 34-246; 36-175; 163-56; 163-227;

## 2329: NERYL PROPIONATE

$C_{10}H_{17}—OOC—C_2H_5$

$C_{13}H_{22}O_2 = 210.32$

For full structure and chemical name – see: Neryl acetate.

Colorless oily liquid. Sp.Gr. 0.92.
B.P. 233° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and very fruity, "jam-like" odor reminiscent of the heavy syrup of fruit preserves, yet with a trace of fresh-floral notes and moderate tenacity.

Intensely sweet-fruity taste in dilution near 10 ppm.

This ester finds a little use in Jasmin bases for its heavy-fruity character, blending very well with the natural "jam"-like character of a Jasmin "chassis"-type. It is also used in Citrus colognes, Rose, Violet, etc. and blends pleasantly with the Ionones, Undecanolide etc. The latter item would also accompany the title ester in Tuberose or Gardenia bases where fruity undertones support the heavy floral notes.

In flavor compositions, the ester finds limited use in berry and fruit complexes at concentrations equal to 5 to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2777.

Prod.: by azeotropic esterification of Nerol with Propionic acid.

33-622; 36-175; 163-56; 163-227;

## 2330: NERYL VALERATE

Neryl pentanoate.
Neryl-*n*-valerianate.
For full structure and chemical name - see: Neryl acetate.

$C_{10}H_{17}$—$OOC(CH_2)_3CH_3$

$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid. Sp.Gr. 0.89.
B.P. 258° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and rich, sweet-herbaceous and fruity odor of good tenacity.

This ester is typical in the series by not being floral, and by having unusual power. Needless to add that if the ester contains traces of free acid, the olfactory picture is completely changed. On the other hand, if it contains unreasonably large surplus of free Nerol/Geraniol mixture, it will be rosy and somewhat floral, rather uninteresting.

The ester could find some use in perfumery as a modifier for Bergamot, Petitgrain, Neroli, Muguet, etc. and it gives very intriguing effects with Vetiver and Oakmoss (Hazelnut-effect) for novel fragrance types.

The title material is *not* listed separately as G.R.A.S. in the American F.E.M.A. list, or by the Federal Register, but it is reasonably safe to assume that the inclusion of the *iso*-Valerate in that list permits the use of the title (*n*-Valerate) ester in food flavors. In such case, we would have another interesting material for "fondant" flavor or soft candy, and a modifier for Bergamot in hard candy flavor.

Prod.: by azeotropic esterification of Nerol with *n*-Valeric acid.

7-298; 33-933; 163-56; 163-227;

## 2331: NERYL-iso-VALERATE

Neryl-*iso*-valerianate.
Neryl-*beta*-methylbutyrate.
For full structure and chemical name - see: Neryl acetate.

$C_{10}H_{17}$—$OOC$—$CH_2$—$CH(CH_3)_2$

$C_{15}H_{26}O_2 = 238.37$

Colorless liquid. Sp.Gr. 0.89. B.P. 252° C.

Insoluble in water, soluble in alcohol and oils.

Rich and sweet-herbaceous, Clary Sage and Hop-type odor with ethereal-fruity notes and good tenacity.

The flavor is primarily "berry-like", remotely reminiscent of Blackcurrant and Apple, quite powerful and pleasant only below 10 ppm.

This ester finds a little use in Rose variations, in Oriental bases, and in Oakmoss blends, where it introduces very attractive sweetness and rich-herbaceous notes. As a modifier in heavy florals it may be used sparingly, but it is not often found in a perfume laboratory.

It finds occasional use in berry, fruit, Apple and "Rose" flavors, and in tobacco flavors.

The concentration is normally as low as 1 to 5 ppm in the finished product.

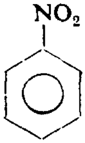
G.R.A.S. F.E.M.A. No.2778.

Prod.: from Nerol by azeotropic esterification with *iso*-Valeric acid.

36-175; 163-57; 163-227;

## 2332: NITROBENZENE

Nitrobenzol.
Mirbane oil.



$C_6H_5NO_2 = 123.11$

Pale yellowish mobile liquid. Sp.Gr. 1.21. B.P. 211° C. Solidifies in the cold, melts at 6° C.

0.2% soluble in water, miscible with alcohol and oils.

Pungent and harsh or offensive, Bitter-almond type odor of poor tenacity. The liquid and the vapors of this material are toxic and irritating to human mucous membranes, skin, eyes, etc. Unquestionable poisoning has occurred in adults, wearing shoes, colored with Nitrobenzene-type dye, in others, using hairdyes containing or liberating traces of Nitrobenzene, etc., etc.

The material is not and should not be classified as a fragrance material. Unfortunately, it has been used as such many years ago and, perhaps up until our days by some unscrupulous "perfume supplier" for various technical or industrial purposes. It has even been used in soap, and experience shows that the most hazardous cases of poisoning occur when Nitrobenzene is *rubbed* into the skin.

Nitrobenzene is included in this work mainly for the above reasons, and also for the interesting fact that its odor resembles that of Benzaldehyde – to a certain degree – which may have a meaning to those who study relationship between chemical structure and odor.

Nitrobenzene is furthermore flammable and its vapors form explosive mixtures with air. This should be reason enough to remove Nitrobenzene definitely and totally from future perfumery raw materials books and from any perfumer's mind, if the material ever was there.

Prod.: by Nitration of Benzene with sulfuric- and nitric acid mixture.

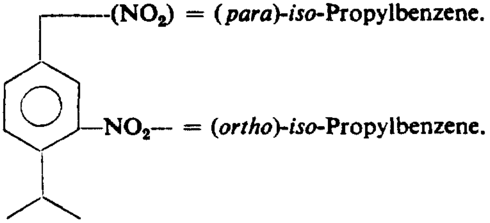
26-626; 34-806; 68-133; 85-91; 95-198; 96-219; 100-724; 159-409; 160-838; 163-57; 163-227; B-V-233;

NOTE: Certain lots of poor grade Bois de Rose oil display a topnote strongly resembling the odor of Nitrobenzene. For a long time this was believed to be caused by contamination from unclean drums at the distilling place. Recent analysis of essential oils reveal that aromatic Nitrocompounds closely related to Nitrobenzene occur naturally in the essential oil from various South American leaves and woods.

See also 2336.

## 2333: NITROCUMENE

The commercial product is normally a mixture of *ortho*- and *para*-Nitrocumene.
Perfumery literature is particularly confusing with respect to the use of the terms -cumene, cumin-, cuminyl- etc. Nitrocumene could thus be: *2*-Nitro-*2*-phenylpropane, or *alpha*-Nitro-*iso*-propylbenzene, but the above isomer-mixture is the one generally referred to.


(NO₂) = (para)-iso-Propylbenzene.
NO₂— = (ortho)-iso-Propylbenzene.

$C_9H_{11}NO_2 = 165.20$

Colorless or pale yellowish liquid.

Practically insoluble in water, soluble in alcohol and oils.

Pungent, but sweet herbaceous-green odor of moderate to poor tenacity.

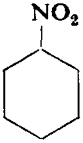
This material has been used in perfume compositions, mainly in soap perfumes, for its power and relative stability, and for its low cost. It could be considered as obsolete, and it is generally avoided in perfumes of today.

Prod.: by Nitration of Cumene, obtained from coal tar.

26-630; 160-938; 163-57; B-V-307, zweiter Ergänzungsband;

## 2334: NITROCYCLOHEXANE

Hexahydronitrobenzene.



$C_6H_{11}NO_2 = 129.16$

Colorless or pale yellowish liquid. B.P. 191° C.

Very slightly soluble in water, soluble in alcohol and oils.

Peculiar, but intensely sweet and pungent-herbaceous odor, displaying a complex of green, anisic, almondy and woody-herbaceous notes. It is probable that the commercial material is far from pure, and thus contains materials of quite different olfactory virtues.

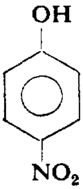
The subject material has been used in soap perfumes but may be considered as abandoned in perfumery. Apart from its hazard of irritation and its moderate toxicity, it does not even offer the perfumer an odor he can be excited about. Rather nondescript.

Prod.: from Cyclohexane by treatment with Nitric acid at 2 to 10 atmospheres pressure (elevated temperature).

67-182; 163-57;

## 2335: para-NITROPHENOL

*1*-Hydroxy-*4*-nitrobenzene.



$C_6H_5NO_3 = 139.11$

Colorless crystals. M.P. 114° C. The material sublimes before melting. Sp.Gr. (liquid) 1.27. B.P. 279° C. (under decomposition).

1.6% soluble in water, 30% soluble in hot water, soluble in alcohol and oils.

Warm-medicinal, sweet "phenolic"-tarry odor of considerable tenacity. The taste is sweet, but burning, and the material is considered moderately toxic.

It has been claimed that a highly purified material is virtually odorless, but the author has his doubts about this.

Although mentioned repeatedly in (older, and a few modern) perfumery literature, this material could be considered as obsolete in perfumery. As a phenol, it causes problems in a composition, and as a nitrated benzene derivative, it is potentially hazardous to human skin.

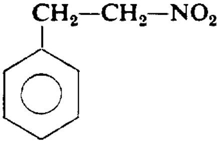
Prod.:

1) Nitration of Phenol gives a mixture of *para*- and *ortho*-Nitrophenol, mainly *para*-. The *ortho*-isomer is volatile with steam and can be almost quantitatively removed from the mixture.
2) by Nitration of *para*-Toluenesulfonic ester of Phenol, followed by hydrolysis is obtained a fairly pure material.

1-453; 26-634; 68-443; 100-729; 160-1158; 163-57; B-VI-226;

## 2336: 1-NITRO-2-PHENYLETHANE

*alpha*-Nitro-*beta*-phenylethane.



$C_8H_9NO_2 = 151.17$

Colorless mobile liquid. B.P. 240° C. Sp.Gr. 1.13.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-floral, warm-spicy and moderately tenacious odor, often described as resembling Cinnamon.

The title material has been mentioned in connection with perfume raw materials, and since it could be made readily available, it has been considered for perfumery purposes.

However, the author feels that the perfumer is extremely well supplied with low-cost, spicy, balsamic, spicy-floral chemicals, and there is little interest in another one, unless it has exceptional virtues.

The title material is not likely to be accepted by the flavor industry and even if it were, it would have competition from low-cost Cinnamal and many excellent floral-spicy flavor materials.

Beyond some academic interest, this material has little new to offer, and the author believes that it may become obsolete within another decade or so. The material has less than 10 years of publicity on its back at this time, and the main interest has been the fact that it represents a very rare group of natural isolates.

Many perfumers have probably wondered why certain lots of "Bois de Rose" oil had such an unattractive "shoe-polish" topnote, and were rejected for perfumery use. There is a possibility that the title material or related Nitro-compounds could be present in minute traces in Bois de Rose oil if contamination took place in collection of plant material. The title material is present (up to 80%) in the essential oils from leaves of trees growing in the same area, where Bois de Rose oil is distilled. An alternative is, of course, that Bois de Rose oil may have been shipped in used, unclean drums, acquiring contamination this way.

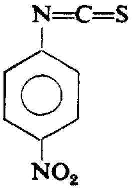
Prod.:

1) from *beta*-Phenylethylamine by oxidation. The amine is obtained from Benzyl cyanide in liquid Ammonia with a Raney-Nickel catalyst, by hydrogenation.
2) by isolation from the essential oil of the leaves of Aniba canellila (in Brazil).

66-105; 66-489; 90-808;

## 2337: 4-NITROPHENYL-iso-THIOCYANATE

"*para*-Nitrophenyl Mustard oil".



$C_7H_4N_2O_2S = 180.19$

Yellowish crystals.

Very slightly soluble in water, soluble in alcohol and oils.

Pungent-sweet herbaceous-spicy odor with resemblance to Bitter-almond and remote similarity to Heliotropine. Good tenacity.

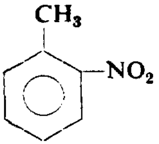
The title material has been used in perfume compositions, including soap perfumes, but the author is of the impression that it is no longer in such use.

There is some academic interest in the material which is related to "Mustard oil", to *para*-Nitrobenzaldehyde, to *para*-Tolyl thiocarbamide (which has an anisic odor) and to *4*-Aldehydo phenylthiocarbimide (which has a more Heliotrope-like odor).

Prod.: from *para*-Nitroaniline with Thiophosgene, or
from *para*-Nitrothiocarbanilide by heating with diluted sulfuric acid.

## 2338: ortho-NITROTOLUENE

*1*-Methyl-*2*-nitrobenzene.



$C_7H_7NO_2 = 137.14$

Yellowish liquid. Sp.Gr. 1.16. B.P. 222° C.

Very slightly soluble in water (0.06%), soluble in alcohol and oils.

Pungent, but very sweet, heavy odor, sweeter than that of Nitrobenzene, and not as offensive. Moderate to poor tenacity.

Although this material is considered much less (perhaps 10 times less) toxic than Nitrobenzene, there is considerable objection to the use of it in modern perfumery. Besides, it does not offer notes which are particularly unusual or unobtainable with other materials. Nitrotoluene may therefore be considered as practically obsolete for such purposes.

Prod.: by Nitration of Toluene. A mixture of (mainly) *para*- and *ortho*-Nitrotoluene is obtained. Separation e.g. by fractional distillation.

26-636; 68-136; 100-732; 160-1252; 163-57; B-V-318;

## 2339: NONADIENAL

This monograph includes:
*trans-2-cis-6*-Nonadienal (from natural Hexenols) – and:
*trans-2-trans-6*-Nonadienal (from synthetic Hexenols).
*) (see odor description at end of monograph).
"Violet leaf aldehyde".
"Cucumber aldehyde".
"Parmantheme" (component).

$$CH_3—CH_2—CH{=}CH—CH_2—CH_2—CH{=}CH—CHO$$

$C_9H_{14}O = 138.21$

Almost colorless or very pale yellowish oil. Sp.Gr. 0.87. B.P. 187° C.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Extremely powerful and very diffusive green-vegetable odor, only in dilution reminiscent (strikingly) of Cucumber or Violet leaf. The taste consists almost exclusively of "olfactory impression", and at concentrations well below 1 ppm it becomes very natural, oily-green Cucumber-like and upon further dilution, buttery-oily.

Although this material has been known and commercially available for nearly 40 years, it still remains a "small" item. And it probably will remain so within perfumery, where its enormous power and very peculiar odor type limits its application to Violet, Cucumber bases (e.g. for handlotions, etc.) and as trace ingredient in new, fresh topnote-compositions, etc. It is interesting in artificial Narcisse.

Its use in flavors is equally limited by its enormous strength, but with the rapid development of packaged and dried foods, there will undoubtedly be increasing need for such natural flavor chemicals to reconstitute lost flavor in processed vegetables, etc.

The material would particularly be used in imitation Cucumber, and as a trace ingredient in many green and fruity flavor types.

It is surprising to notice, that this aldehyde is *not* listed as G.R.A.S. by the American authorities, although the corresponding alcohol is so. The present (1968) market price is U.S. $ 2500.— per kilo.

*) Prod.: most methods start from *3*-Hexenol. The natural Hexenol will yield *trans-2-cis-6*-Nonadienal which has a sweeter, creamier and more attractive, natural-oily note in proper dilution.

The synthetic Hexenol yields *trans-2-trans-6*-Nonadienal, which has a more dry and sharp odor, even at the same dilution. The former (natural type) isomer is the preferred one.

1) via Hexenyl iodide and its Grignard compound, with Acrolein to the carbinol. By treatment with Phosphorous tribromide and saponification is obtained the alcohol Nonadienol which can be oxidized to the title aldehyde by Chromic acid oxidation.
2) from Dipropargyl via Octadi-yne to Nonadiynal-diethylacetal, followed by selective hydrogenation to Nonadienal diethylacetal (see next) which yields the title aldehyde by acid hydrolysis.

Several other methods are known and used.

1-171; 5-329; 5-347; 34-1210; 89-43; 156-25; 159-443; 163-57;

Sample: Compagnie Parento – and: Haarmann & Reimer.

## 2340: NONADIENAL DIETHYLACETAL

$CH_3—CH_2—CH{=}CH—CH_2—CH_2—CH$
$=CH—CH(OC_2H_5)_2$

$C_{13}H_{24}O_2 = 212.34$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, fresh-green Cucumber odor, less oily and, in proper dilution, much fresher and lighter than the odor of the aldehyde itself (see previous monograph).

This acetal is occasionally used in perfume compositions as a modifier for the aldehyde. It is more versatile because it is generally fresher, not distinctly oily-vegetable, and its green notes can be used in novel Citrus topnote-compositions, and it also works well with Galbanum and Oakmoss in fruity-aldehydic "modern" fragrance types.

The acetal could find use in flavor compositions if it were permitted, but it is not specifically listed as G.R.A.S. by the American authorities.

Prod.: several of the manufacturing methods for the aldehyde rely upon the production of the acetal from which the aldehyde is subsequently liberated. See under "Prod.:" in monograph preceding this.

Sample: Compagnie Parento, Inc.

## 2341: NONADIENOL

*trans-2-cis-6*-Nonadienol (natural and preferred type).
*trans-2-trans-6*-Nonadienol (synthetic and less desirable type).
*) See note below under "Prod.:".
"Violet leaf alcohol".
"Cucumber alcohol".
The monograph includes the two above mentioned isomers. Two other isomers are known, but not commercially interesting.

$CH_3—CH_2—CH{=}CH—CH_2—CH_2—CH$
$=CH—CH_2OH$

$C_9H_{16}O = 140.23$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 196° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Extremely powerful and very diffusive oily-green, herbaceous and, in proper dilution, sweet, pleasant leafy-vegetable odor of moderate to poor tenacity.

Sweet cucumber-peel, vegetable-green taste in concentrations near 0.1 ppm or lower.

This alcohol, identified in natural products, is commercially available (at approximately U.S. $ 2500.— per kilo) and has been used for the past 30 years in minute traces in Violet perfumes, Narcisse bases, and in topnote compositions as a green-fresh, natural and very diffusive note. The material is also used in the revived "Cucumber" odor for hand-lotions, etc. Interesting effects are achieved with this material in Muguet, Lily, Cyclamen, Ylang-Ylang, etc.

Much more frequently used in flavor compositions, the title alcohol is almost a "must" in Cucumber imitation, in many berry flavors and "green-Apple", fruit complexes and the old-fashioned "Violet" flavor with Ionones, Geranium oil, etc.

The concentration in finished products is normally as low as 0.01 to 0.05 ppm – one to five parts in one hundred million parts of consumer product. Which of course compensates for the very high cost of this chemical (the aldehyde is equally expensive).

With the explosive development of modern food packaging, dried foods and vegetables, desserts, etc. it is very probable that chemicals such as this may become everyday items on the flavorist's shelf.

G.R.A.S. F.E.M.A. No.2780.

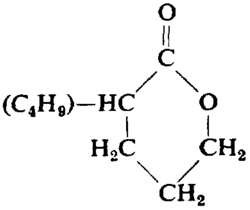
*) Prod.: (see Nonadienal). When natural Hexenol is used as a starting material, the preferred isomer (see above) will result. This is called "natural" because it is evidently identical to the naturally occurring alcohol. If synthetic Hexenol is used, the less desirable isomer will result. It has a more dry, less pleasant-oily character. There are several methods in use for the production of this alcohol.

5-329; 5-347; 34-1210; 87-488; 140-126; 156-16; 163-57;

Sample: Compagnie Parento and: Haarmann & Reimer, GmbH.

## 2342: delta-**NONALACTONE**

*alpha-n*-Butyl-*delta*-valerolactone.
Nonanolide-*1*:*5*.



$C_9H_{16}O_2 = 156.23$

Colorless very viscous liquid. Sp.Gr. 0.99.

Almost insoluble in water, soluble in alcohol and oils.

Very powerful, fatty-oily, but rich and sweet, mildly nut-like odor of excellent tenacity.

Fatty-milky-creamy taste with mildly nut-like, oily-buttery character. The pleasant taste level is well below 10 ppm, unless other flavor materials are present.

The title lactone, an isomer of the well-known "aldehyde C-18" ("Coconut")*) has become commercially available and is finding use in perfume compositions as a modifier for Nonalactone ("Coconut aldehyde") e.g. in heavy floral bases, where the creamy effect is definitely desirable, Gardenia, Tuberose, Jasmin, etc.

The chief interest, however, is in flavors. The title lactone may introduce natural and inimitable effects in milk, butter, cream and particularly in nut flavors.

The Japanese manufacturer recommends 1 to 5 ppm in milk and beverages, 2 to 10 ppm in ice cream, and 5 to 20 ppm in baked goods.

Prod.: e.g. from *delta*-Hydroxy nonoic acid.

157-297;

Sample and data: Soda Aromatic Co., Ltd., Japan, Sept. 1967.

*) this isomer is listed under Nonanolide in the present work. (No. 2350).

## 2343: n-NONANAL

*n*-Nonyl aldehyde.
Aldehyde C-9.
Nonanoic aldehyde.
Pelargonic aldehyde.
Pelargonaldehyde.
Nonoic aldehyde.
*alpha*-Oxononane.

$CH_3(CH_2)_7CHO$

$C_9H_{18}O = 142.24$

Colorless oily liquid. Sp.Gr. 0.83.
B.P. 191° C.

Solidifies in the cold, melts again at 6° C.

Practically insoluble in water, soluble in alcohol and oils.

Very powerful and diffusive fatty-floral, waxy odor of moderate tenacity. In proper dilution, the fatty notes become more pleasant, floral-waxy, more rosy and sweet, fresh as Neroli.

The taste in concentrations below 5 ppm is refreshing, citrusy, waxy.

This aldehyde is used very extensively, but also very sparingly in volume, in perfume formulations. Trace amounts, often less than 0.1%, are used in Rose, Lily, Peony, Orris, Geranium, Citrus, Orangeblossom, Jasmin, Tuberose, Opopanax and many other fragrance types. The aldehyde will supply very natural "flower-wax" or "petal"-notes, and give tremendous "lift" to a perfume. It often forms part of an "aldehydic base" which in turn may form part of a topnote composition.

In flavor compositions, the aldehyde is used for imitation Citrus, particularly Lemon and Mandarin. Concentrations are very low, normally about 0.2 up to about 6 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2782.

Prod.:

1) from Oleic acid or from Castor oil via Undecylenic acid.
2) by catalytic oxidation of *n*-Nonanol.

5-77; 26-646; 31-31; 34-806; 89-25; 106-34; 140-158; 156-22; 163-57; B-I-708;

## 2344: NONANAL DIETHYLACETAL

*9,9*-Diethoxynonane.
*n*-Nonylaldehyde diethylacetal.
Pelargonaldehyde diethylacetal.

$CH_3(CH_2)_7CH(OC_2H_5)_2$

$C_{13}H_{28}O_2 = 216.37$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Delicately green-oily, mildly herbaceous-floral odor of good tenacity. Materials from different suppliers may show considerable difference in odor, and traces of free aldehyde will strongly influence this olfactory picture.

This acetal, although very well known, is only rarely used in perfumes. The amount of Nonanal needed in a fragrance is so small that its dilution usually ensures good stability, and there will be no need to use the acetal as a substitute for the aldehyde. However, the pure acetal has an odor of its own, not nearly as fatty-waxy as that of the aldehyde, and it would be a good idea to try out this acetal before "discarding" it as a "replacement for Nonanal", which it is not.

Particularly interesting are the effects in modern topnote compositions e.g. with Galbanum or with Estragon, Basil, Hyssop or Geranium. It is also interesting as a companion to the newer unsaturated olefinic aldehydes, and it works very well with Violet leaf absolute, etc.

Prod.: by condensation of Nonanal with Ethyl alcohol.

B-I-708;

## 2345: NONANAL DIMETHYLACETAL

*n*-Nonylaldehyde dimethylacetal.
Aldehyde C-9, dimethylacetal.
Pelargonaldehyde dimethylacetal.
9,9-Dimethoxynonane.

$CH_3(CH_2)_7CH(OCH_3)_2$

$C_{11}H_{24}O_2 = 188.31$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing and relatively powerful citrusy-floral, oily-green odor of moderate tenacity. Traces of free aldehyde tend to dominate the overall odor.

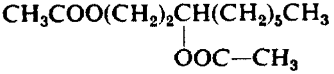
Since the odor characteristics of this acetal are fairly close to those of the aldehyde itself, there has not been much interest in the dimethylacetal. Perhaps the commercial products have been rather impure, or poorly stable. Only an aldehyde-free acetal has something specific to offer, and it is apparently not enough to make it a common commercial item.

Prod.: *from* Nonanal by condensation with Methanol.

37-281;

## 2346: NONANE DIOL-1 : 3-ACETATE

The title material is the chief or the major component of a large number of specialties, marketed under a wealth of trade names:
Nonane diacetate,
Drago-Jasimia,
Jessemal,
Jasmonyl,
Ysminia,
Jasmelia,
Diasmylacetate.
Diasmol.
"Octylcrotonyl acetate".
Hexylene glycol diacetate.
Tepyl acetate, etc., etc.
Other components in most of these products are:
Decane diol mono- and diacetates,
Nonane diol monoacetate and various Pyran-derivatives, including Tetrahydropyranyl ethers. The latter is the chief component of some of the above specialties, and it is sold in an almost pure state under other trade names.



$$\begin{array}{l} CH_3COO(CH_2)_2\underset{\displaystyle OOC-CH_3}{\underset{|}{C}}H(CH_2)_5CH_3 \end{array}$$

$C_{13}H_{24}O_4 = 244.34$

Colorless, slightly oily liquid. Sp.Gr. about 0.97.

Slightly soluble in water, soluble in alcohol and oils.

Powerful, oily-herbaceous, warm odor of moderate tenacity. Considerable variations are observed when studying the various brands. Notes of floral-Jasmin character, mushroom-like Lavender character or almost caramellic sweetness may be present, predominant or absent in one or the other specialty.

The title material is intended to be a Jasmin base material. It can introduce the oily-herbaceous undertones, characteristic of Jasmin absolute, but not available from one single chemical. It is used very widely for that purpose at concentrations from 1% up to 5% or in exceptional cases higher. It is very popular in soap perfumes where its stability and diffusive power increase the "odor value" of the soap fragrance.

Some of the specialties claim to be exclusively "floral", while the general impression is that of truly oily-herbaceous character. In fact, many of the above specialties perform well in Lavender compositions. It depends largely upon the accompanying chemicals. With Amylcinnamic aldehyde and Benzylacetate, the Jasmine tone has already been founded, while with Linalool-Ethyllinalool-Linalylacetate and good terpenes, a Bergamot-Lavender base has been laid down, and in both cases the note will be pleasantly supported and enhanced by the title material (or the specialty).

This material is also used in flavor compositions, and its effect in berry complexes or fruit blends is quite interesting. The concentration is usually very low, because it is a powerful flavor, perceptible well below 1 ppm. From 0.3 to 1.5 ppm is normal in finished products.

G.R.A.S. F.E.M.A. No.2783.

Prod.: most methods are based upon *1*-Octene as a starting material, but there are countless variations in the processes.

The most important point in the process is that of selecting the fractions from the vacuum-distillation of the reaction mixture. Odors from harsh-metallic-terpeney through musty-fungoid to sweet oily and floral appear throughout the distillation, and the differences in appreciation on the part of the controlling perfumer determines the odor type of the final product.

A few suppliers have realized that there are differences of opinion, and that various sections of the distillation have entirely different characteristics.

A typical example is I.F. & F.'s "Jessemal" which is the regular product in competition with numerous others.

A new type, called "Jasmal" represents an entirely different section of the distillation and offers a particularly "jasminy" chemical with the warm-herbaceous, almost tea-like note. Firmenich's "Ysminia" is equally refined towards the Jasmin theme, and so is "Hyxis" of de Laire, a composition in which the title material plays a somewhat minor role.

U.O.P. Chemical Company's "Tepyl acetate" is named after one of the chief components, Tetrahydropyranylacetate, but it is also a complex mixture of many active olfactory ingredients.

The title material (the composite of specialties) represents a typical and interesting example of achievements in that part of modern perfume chemistry which is *not* based upon findings in natural products.

106-215; Samples and data from numerous suppliers.
See also monograph: *5*-Methyl-*3*-butyl tetrahydropyran-*4*-yl acetate (= Tepyl acetate, so-called). No. 1935.

## 2347: NONANOIC ACID

Nonoic acid.
Pelargonic acid.
*n*-Nonylic acid.
Octane-*1*-carboxylic acid.

$CH_3(CH_2)_7COOH$

$C_9H_{18}O_2 = 158.24$

Slightly viscous or oily, colorless liquid, solidifying in the cold, melting again at 13° C. The solid material appears as leafy, colorless or shiny white crystals. Sp.Gr. 0.91 (liquid). B.P. 256° C.

Very slightly soluble in water, soluble in alcohol and oils.

The pure chemical has a mildly nut-like, fatty and acid odor of good tenacity. If the impurities include unsaturated compounds, there may be developed repulsive off-odors, rancid notes, etc. which are not characteristic of the title acid.

The taste is quite powerful, waxy-nut-like, in extreme dilution not sour, but slightly brandy-like.

This acid finds some use in perfume compositions for its supporting effect in Orris (with Ionones), and as a component of artificial essential oils.

It is also used in minute amounts in flavor compositions, such as berry complexes, fruit, nut and spice blends and in Cognac or Brandy imitation (mainly with esters of the acid).

The concentration used is normally about 1 to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2784.

Prod.:
1) by oxidation of Oleic acid.
2) by malonic ester synthesis, from Heptyl iodide.

Castor oil may be the basic raw material in both cases.

26-646; 66-564; 90-92; 106-281; 140-142; 160-1140; 163-61; B-II-352;

## 2348: NONANOL-1

Nonyl alcohol.
Alcohol C-9.
*l*-Nonanol.
Octyl carbinol.
Pelargonic alcohol.
"Nonalol".

$CH_3(CH_2)_7CH_2OH$

$C_9H_{20}O = 144.26$

Colorless oily liquid. Sp.Gr. 0.83.
B.P. 213° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, oily-floral, fresh and "petal"-like odor, rather fatty when undiluted, light and almost rosy when highly diluted.

Oily, but at concentrations near 1 ppm refreshingly citrusy-sweet taste.

This alcohol is used quite frequently, although always at very low concentration, in perfume compositions, mainly floral and citrusy types. It contributes freshness to Rose, waxy-"petal"-notes to Jasmin and Neroli, delicate floral tones to Peony, etc. Some perfumers find that its odor resemble that of Citronellol, but there is considerable difference of power, and there is often good use for both materials in the same composition.

Traces of this alcohol are used in flavor compositions, e.g. imitation Butter, Peach, Pineapple, Orange (and other citrus types), etc.

The concentration may be as low as 0.5 ppm in the finished product, or as high as 20 ppm in the case of chewing gum.

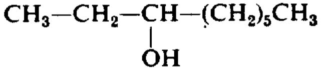
G.R.A.S. F.E.M.A. No.2789.

Prod.:
1) from Heptaldehyde via Heptanol and Heptylmagnesiumbromide with Ethylene oxide to the alcohol.
2) by reduction of Ethylpelargonate.

5-15; 31-23; 34-806; 31-16; 66-314; 100-734; 106-27; 160-1126; B-I-423;

## 2349: 3-NONANOL

Ethyl hexyl carbinol.



$$CH_3{-}CH_2{-}\underset{\displaystyle OH}{\underset{|}{CH}}{-}(CH_2)_5CH_3$$

$C_9H_{20}O = 144.26$

Colorless liquid. B.P. 206° C. Sp.Gr. 0.86.

Very slightly soluble in water, soluble in alcohol and oils.

Herbaceous, mildly spicy-earthy, but overall sweet and oily odor of moderate to poor tenacity. The odor is not floral like the *l*-Nonanol, and not "mushroomy" like Vinyl hexyl carbinol. It is also less fruity than the Methyl heptyl carbinol (*2*-Nonanol). In brief, the odor is probably the least natural of all the common Nonanols and related alcohols.

The title material has been used in perfume compositions mainly because it was inexpensive, derived from a large-scale manufactured industrial chemical, but it has also served as intermediate in the manufacture of a number of new perfume chemicals, including the hydroxylated alcohols for Lavender and Jasmin type odors.

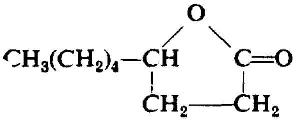
As long as this material is available at a very low cost, it can probably find use in low-cost detergent perfumes, etc. as supporting note for fresh-herbaceous fragrances, for odor power and in fantasy fragrances.

Prod.: by hydrogenation of Ethyl hexyl ketone.

It can also be prepared by reduction of Hexyl vinyl carbinol.

# 2350: NONANOLIDE-1:4

*gamma*-Nonalactone.
*gamma-n*-Amyl butyrolactone.
*4*-Hydroxynonanoic acid, lactone.
"Aldehyde C-18" (so-called).
"Coconut aldehyde".
"Prunolide".
"Abricolin".
*gamma*-Pelargolactone.
*gamma*-Nonyllactone.



$C_9H_{16}O_2$ = 156.23

Colorless or very pale straw-colored oily liquid. Sp.Gr. 0.97. B.P. 243° C.

Practically insoluble in water, soluble in alcohol and oils.

Creamy, coconutty, delicately fruity (in extreme dilution) and floral-musky odor of excellent tenacity.

Creamy-nut-like taste at concentrations near 50 ppm, delicately fruity and sweet at 1 to 5 ppm.

This material is one of the most frequently used lactones in perfumes and flavors. Its field of application reaches from the finest luxury perfumes to inexpensive masking odors, from Gardenia flower bases to Coconut candy flavors, etc. etc. Its intense sweetness and tenacity is often utilized along with that of Undecanolide (so-called Aldehyde C-14) in Gardenia, Tuberose, Honeysuckle, Stephanotis, Plumeria, Jasmin and many other heavy floral types. Modern fantasy perfumes with emphasis on musk and lactones may include the title material and produce unusual fixative effect of overwhelming sweetness, and novel versions of Oriental fragrance types can be made with Sandalwood, Styrax and the title lactone as part of the base. Its power is often underestimated by the perfumer (if he has no experience as a flavorist) and the lactone will "grow" out of the perfume and unpleasantly dominate the fragrance.

In flavors, the lactone finds even more extensive use, and often in much higher concentration. Besides Coconut, this material is used in imitation Bitter-almond, in fruit blends (fixative), berry complexes, nut variations, American Cherry flavor, etc. the concentration may vary from 10 to 50 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2781.

Prod.:

1) from Methylacrylate plus Hexanol with Di-*tertiary*-butylperoxide.
2) from Undecylenic acid with Malonic acid condensation.
3) from Nonenoic acid by Lactonization.

Nonenoic acid may be obtained from Castor oil – Heptanal, with Malonic acid and Pyridine to Nonenoic acid.

5-206; 31-173; 41-41; 90-658; 106-43; 140-153; 156-226; 159-419;

# 2351: 3-NONANONE

Ethyl hexyl ketone.
Hexyl ethyl ketone.

$CH_3$—$CH_2$—CO—$(CH_2)_5CH_3$

$C_9H_{18}O$ = 142.24

Colorless liquid. Sp.Gr. 0.84. B.P. 190° C.

Practically insoluble in water, soluble in alcohol and Propylene glycol, miscible with oils.

Powerful and, when undiluted, somewhat sharp or pungent grassy-herbal odor with green-fruity undertones. Upon dilution the herbal notes become more natural-sweet, mildly oily, remotely mushroomy-earthy, warm.

This ketone has only recently become a common commercial item in a satisfactory state of purity. It has been suggested for use in perfume compositions and in artificial essential oils.

Its green-fruity notes are useful in Jasmin, Lavender, Lily and its mildly oily-earthy character blends well into Oriental or Opopanax notes, etc. and the material offers interesting modifications of the Lavender theme where it blends very well with Oakmoss and Amylsalicylate. Discrete amounts give power and natural notes in artificial Lavender.

Prod.:
1) by heating of Propionic and Heptanoic acids over Thorium oxide at 450° C.
2) by hydrogenation of Ethyl hexyl carbinol (*3*-Octanol).

160-1126;

## 2352: 3-NONANON-1-YL ACETATE

Methylol methyl hexyl ketone acetate.
"Ketone alcohol ester".

$CH_3(CH_2)_5CO—CH_2—CH_2—OOC—CH_3$

$C_{11}H_{20}O_3 = 200.28$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Herbaceous-fruity, warm-ethereal odor of moderate tenacity.

This *beta*-Ketol ester has been suggested for use in perfumes and flavors. It is mostly used in flavors.

Its herbaceous character offers interesting notes for Lavender and Fougère types, and it blends very well with the spicy versions of Men's fragrances, etc.

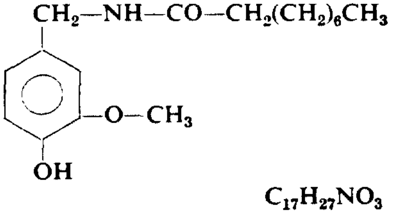
It is also used in fruit and spice flavor compositions to introduce a richer herbaceous and more "natural" character. The concentration used is about 1 to 10 ppm, sometimes even less, in the finished product.

Prod.: by condensation of Methylhexylketone with Formaldehyde under mildly alkaline conditions. The resulting *beta*-Ketol is subsequently acetylated.

G.R.A.S. F.E.M.A. No.2786.

## 2353: NONANOYL VANILLYLAMIDE

Pelargonyl vanillylamide.
*N*-(*4*-Hydroxy-*3*-methoxybenzyl)nonanamide.
*N*-Nonanoyl-*4*-hydroxy-*3*-methoxybenzylamide.



$C_{17}H_{27}NO_3 = 293.41$

White powder.

Slightly soluble in water, soluble in alcohol and oils.

Practically odorless.

Pungent, burning taste or, at first apparently tasteless, but a burning sensation with typical peppery pungency appears in the back of the mouth. The pungency is perceptible at concentrations below 1 ppm, but the title material is not nearly the most pungent of the series. The normal use concentration is about 10 ppm in the finished product.

A large number of vanillylamines, derivatives with saturated or unsaturated acids, are known. The pungent principles in Capsicum and Black Pepper contain such derivatives. The next higher homologue with an unsaturated chain is the pungent principle of Capsicum.

The title material is used in spice flavors to increase pungency without changing the flavor as such (no odor change). It has the advantage of being white (colorless) which sometimes is of importance where spice extracts introduce too much color.

It is interesting for those who study correlation between taste and chemical structure to notice the relationship between the various pungent derivatives, and the difference in the taste of the nitrogen-free members (e.g. Zingerone, etc.) most of which are not pungent at all.

G.R.A.S. F.E.M.A. No.2787.

Prod.: from Nonanyl chloride plus Vanillylamine.

158-209;

See also: 159-308; see monograph: Capsaicin. (567).

## 2354: 3-NONANYL ACETATE

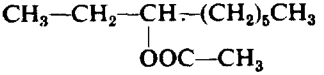
Ethyl hexyl carbinyl acetate.

Do not confuse with:

*3*-Nonenyl acetate, or

*3*-Nonanon-*1*-yl acetate.

See both monographs.



$$\begin{array}{l} CH_3{-}CH_2{-}\underset{\displaystyle OOC{-}CH_3}{\underset{|}{CH}}{-}(CH_2)_5CH_3 \end{array}$$

$C_{11}H_{22}O_2 = 186.30$

Colorless oily liquid. B.P. 225° C.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing, fruity-floral odor with a dry-waxy, pleasant note and moderate tenacity.

The title material, although not immediately reminiscent of any natural material, is quite versatile in use. It will freshen-up a Rose or a Lavender, give power to a Fougère and take the nauseating sweetness out of Amylsalicylate, give interesting nuances in Citrus fragrances, and it is a challenging base for new fantasy notes.

Occasionally, the material is plentiful and inexpensive, since it is derived from an industrial chemical, but it is not often offered from the regular manufacturers of perfume chemicals.

Prod.: by azeotropic esterification of *3*-Nonanol with Acetic acid.

## 2355: NONANYL PIPERIDINE

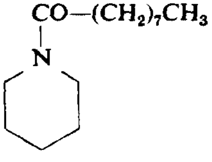
Nonanoyl piperidine.

Pelargonyl piperidine.

(The title name, a commercial name, is slightly confusing).

Pelargonic acid, piperidide.

Pelargonic piperidide.



$C_{14}H_{27}NO = 225.38$

Colorless or pale straw-colored liquid.

B.P. 260° C.

Very slightly soluble in water, soluble in alcohol and oils.

Practically odorless when pure, but causes a violently burning taste sensation, even at very low concentration.

This material has been suggested for use in flavor compositions as a colorless substitute for Black Pepper or Pepper extracts (Oleoresin). It may also be used in place of Capsicum for pungent effect.

Out of many known and commercially available acyl piperidides, the title material is one of the most pungent, and it is comparatively easy to manufacture.

See also monographs on Capsaicin (567) and Nonanoyl vanillylamide (2353).

Prod.: from Piperidine and Nonanylchloride.

159-304;

## **2356: 2-NONENAL**

*2*-Nonen-*1*-al.
*beta*-Hexylacrolein.
*3*-Hexyl acrolein.
"Iris Aldehyde" (L. Givaudan & Co.).
*alpha*-Nonenyl aldehyde.
*alpha-beta*-Nonylene aldehyde.
Heptylidene acetaldehyde.

$C_6H_{13}—CH{=}CH—CHO$

$C_9H_{16}O = 140.23$

Almost colorless or very pale straw-colored, oily liquid. Sp.Gr. 0.86. B.P. 189° C.

Insoluble in water, soluble in alcohol and oils.

Extremely powerful and diffusive, penetrating, fatty-orrisy odor in higher concentrations. In dilutions below 0.1% the odor becomes more Orris-like, waxy, less fatty, slightly green and in extreme dilutions quite pleasant.

The aldehyde oxidizes very easily in air (to Nonenoic acid).

This aldehyde, for many years available only from one source, is slowly becoming popular as a trace additive to Ionones, Methylionones, to lend power and diffusion to woody-orrisy notes in soap perfumes, waxy-petal-like notes to floral fragrances, etc.

The concentration in a perfume oil may be of the order of magnitude of 0.01 to 0.03%. An addition of 0.02% of this aldehyde to a normal grade of "*gamma*"-Methylionone will produce a distinctly ("orrisy") perceptible effect, desirable and attractive in the opinion of many perfumers.

It is interesting to note that a chemical called Nonenyl nitrile has a very similar odor, and was developed in the search for a material of said odor and with better stability in air and mild alkali. However, the subject aldehyde seems to perform quite well in soap, presumably because of the extreme dilution which physically protects the aldehyde to a certain degree.

Prod.:

1) by oxidation of Nonenol.
2) by condensation of Acetaldehyde and Heptaldehyde in the presence of a catalyst.

Note: The very limited literature on this subject brings rather wide variations in the odor description. It could be due to the evaluation of partially deteriorated samples by some observers.

163-57; 4-61; 86-59; 89-42; 156-26; Givaudan data; See also: Nonenyl nitrile (2362).
Samples: Givaudan Corp. and Compagnie Parento, Inc.

## **2357:** omega-**NONENOL**

*8*-Nonen-*1*-ol.
*omega*-Nonenyl alcohol.

$CH_2{=}CH(CH_2)_6—CH_2OH$

$C_9H_{18}O = 142.24$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and very diffusive, waxy-floral odor with balsamic-nutty note and moderate tenacity.

The floral note is not distinctly rosy, nor does it resemble any other flower, and this may be one of the reasons for the lack of acceptance of the title alcohol. The balsamic notes resemble a fortified Opopanax and invite to experiments with Oriental bases, while the "nutty" note encourages the use of Oakmoss with this alcohol.

The material is rarely found commercially available, and it may be comparatively expensive to manufacture in an acceptable grade.

The next higher homologue, *omega*-Decenol is listed in this work, and is known under the trade name "Rosalva" (I.F.& F.).

## 2358: NONEN-5-ONE-2

"Hexenylacetone".
Methyl heptenyl ketone.

$$\mathrm{CH_3{-}CH_2{-}CH_2{-}CH{=}CH{-}CH_2{-}CH_2{-}CO{-}CH_3}$$

$$\mathrm{C_9H_{16}O} = 140.23$$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, refreshing, green-oily, herbaceous odor of moderate to poor tenacity.

This ketone, an isomer of "Ethylheptenone", has been suggested for use in perfume compositions, where its power and herbaceous freshness could give lift to Lavender, Chypre, Citrus or Oriental fragrance types.

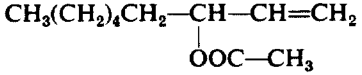
The material is rarely offered under its proper chemical name, but it is the author's impression that even the various trade names covering this item, are rather limited in use.

Prod.: (several methods) e.g. by hydrolysis of *2*-Hexenyl-acetoacetic ester.

See also monograph: Ethyl heptenone (Methyl ethyl hexenone).

## 2359: 3-NONENYLACETATE

Hexyl vinyl carbinyl acetate.
"Andryl acetate" (The alcohol is also called "Androl").



$$\mathrm{CH_3(CH_2)_4CH_2{-}\underset{\substack{|\\ OOC{-}CH_3}}{CH}{-}CH{=}CH_2}$$

$$\mathrm{C_{11}H_{20}O_2} = 184.28$$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

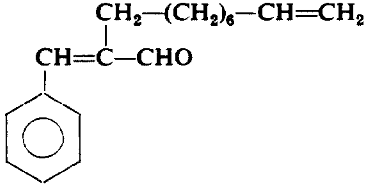
Powerful, earthy-herbaceous, in dilution refreshingly spicy-herbal odor of moderate tenacity.

This ester, a higher homologue of the Amyl vinyl carbinyl acetate known from Lavender oil, has recently become a commercial item. Available at a very attractive price, and considering the power of the material, it should have good possibilities as a modifier and "renforcateur" in all herbaceous fragrances, Lavender, Lavandin, Fougère, Chypre, Colognes, Clary Sage, etc. It gives very interesting effects with Opopanax and Patchouli for novel "Oriental" themes, and it may add the desirable herbaceousness to heavy floral fragrances such as Jasmin and Gardenia.

Prod.: by acetylation of the alcohol, which is obtained from Hexylmagnesium bromide plus Acrolein.

Sample: Takasago Perfumery Company, Ltd., Tokyo, 1967.

## 2360: alpha-NONENYL CINNAMIC ALDEHYDE



$$\mathrm{C_{18}H_{24}O} = 256.39$$

Pale yellowish oily, slightly viscous liquid. Sp.Gr. 0.95. B.P. 306° C.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol.

Vegetable-green, mildly oily-herbaceous odor of considerable tenacity. The odor is sometimes described as resembling Artichoke (Cynara scolymus).

The development of this "sophisticated" chemical is apparently a result of an experiment based upon hopes that the combination of "Aldehyde C-11" (Undecy*lenic*) would give an interesting condensation product with

Benzaldehyde in the process used to make the very successful Amylcinnamic aldehyde.

But the title material reached very few shelves and is known by very few perfumers. And it is not missed by many. Its extremely high boiling point causes some problems in producing a uniform quality and obtaining a reasonable yield. And its odor type does not make the material as versatile as the lower members of this series.

It would be reasonable to say that the title aldehyde is practically obsolete in perfumery.

Prod.: by condensation of Benzaldehyde with *10*-Undecenal.

93-150;

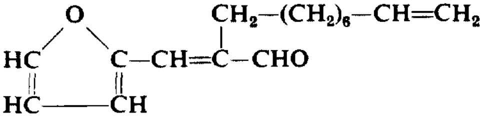
NOTE: *alpha-n*-Nonyl cinnamic aldehyde which is made from Unde*cylic* aldehyde and Benzaldehyde, is known, but practically odorless and of no apparent interest to the perfumer.

## 2361: alpha-NONENYL FURFURACROLEIN

The title name is incorrect.

*alpha*-Nonenyl-*3*-(*2*-furyl)-propenal (chemically correct name).

*alpha*-Nonenyl-*beta*-*2*-furylacrolein.



$C_{16}H_{22}O_2 = 246.35$

Pale yellowish liquid.

Insoluble in water, soluble in alcohol and oils.

Faint, but pleasant, warm-woody-herbal odor with some resemblance to Ambregris. Excellent tenacity but rather poor stability.

This material, very rarely offered commercially, has probably little more than academic interest, since many materials with good Ambregris odor have been developed after the first mention of this peculiar aldehyde.

It was probably hoped that a condensation product of such powerful and useful odorants as Undecylenic aldehyde and Furfural would yield something really interesting. But it did not. Fortunately, chemistry has often shown us that powerful and interesting odorants can be prepared from odorless or olfactorily uninteresting starting materials.

Prod.: by condensation of Furfural with *10*-Undecenal under mildly alkaline conditions.

31-40;

## 2362: NONENYL NITRILE

*2*-Noneoic nitrile (correct name).

*1*-Octenylcyanide.

$CH_3(CH_2)_5CH{=}CH{-}CN$

$C_9H_{15}N = 137.23$

Colorless or almost colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

This Nitrile was developed when interest was shown in *2*-Nonenal, the corresponding aldehyde. With the greater stability in perfume compositions of Nitriles over the Aldehydes, it was expected that the Nitrile would be a superior replacement for the aldehyde. The odor of the Nitrile, however, although resembling that of the Aldehyde, is less waxy-fatty, more sharp-pungent than that of the aldehyde. It would probably serve the two materials better if they were not compared so closely. They both have a mission in modern perfume compositions.

The title Nitrile is offered under various trade names, but the main difficulty in promoting it as a fragrance material is its enormous power. It is best demonstrated as a trace additive to an already known composition, or to a well-known perfume chemical, e.g. Methylionone. For novel effects in the classical "aldehydic" topnote compositions, this material has interesting possibilities.

Normal use-concentration may be as low as 0.05%, which, after all, is slightly higher than the normal level for the aldehyde. It shows once more that the human nose is notoriously poor when it comes to comparison of odor strength – for the title Nitrile is generally advertised as being stronger than the aldehyde. A very subjective problem.

Prod.: *from* 2-Octenoic bromide plus Potassium cyanide.

Other methods are known.

## 2363: NONYL ACETATE

*n*-Nonyl ethanoate.
Pelargonyl acetate.
Acetate C-9.
Nonanol acetate.

NOTE: Commercial grades may include Di-*iso*-butyl carbinyl acetate, and the reader may also consult the monographs on:
*secondary*-Nonyl acetate, under which the isomer Ethyl hexyl carbinyl acetate is mentioned. The commercially available *iso*-Nonyl acetate is listed in this work under:
*3,5,5*-Trimethylhexylacetate.

The perfumery literature shows considerable inconsistency in the nomenclature of Nonyl acetates.

(Title material): $CH_3(CH_2)_8—OOC—CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Sp.Gr. 0.88. B.P. 212° C.

Practically insoluble in water, soluble in alcohol, miscible with oils. Fairly soluble in Propylene glycol.

Powerful fruity-green, leafy and mildly earthy odor of moderate to poor tenacity.

This ester, although rarely used in volume, finds application in numerous types of fragrance: Orangeblossom, Rose, Gardenia, Lavender, Violet, Oriental, Opopanax, Orris, Citrus (Lemon in particular), etc.

Its refreshing note blends equally well in floral and non-floral types, since it emphasizes Violet in the presence of Ionones, greenness in presence of Galbanum, etc. Its low boiling point should be kept in mind, since the material demands considerable fixation in order to perform pleasantly and not "stick out" in the initial note of the fragrance.

The ester finds some use in flavor compositions for imitation Apricot, Peach, Lemon and other Citrus types, fruit complexes, etc. Its sweet-fruity taste is accompanied by a "peel"-like freshness, and the material is quite powerful. Concentrations vary from 1 to 3 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2788.

Prod.: by azeotropic esterification of *n*-Nonanol with Acetic acid – or by ordinary Acetylation with Acetic anhydride.

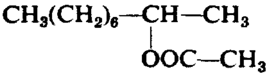
33-503; 41-15; 28-652; 100-734; 106-18; 140-135; 163-57; B-II-135;

## 2364: secondary-NONYL ACETATE

*2*-Nonanol acetate.
Methyl heptyl carbinyl acetate.

NOTE: The perfumery literature will often refer to the isomer: Ethyl hexyl carbinyl acetate = *3*-Nonanol acetate (103-201), but the author of this work has chosen to describe the title material (*2*-Nonanol acetate) since the corresponding alcohol is an important flavor chemical and has been identified in Nature, while the *3*-Nonanol acetate does not seem to occur in important natural products or have significance in flavor creation. That material appears under a separate monograph in this work. (See 2354).

Title material:



$$CH_3(CH_2)_6—\underset{\displaystyle OOC—CH_3}{\underset{|}{CH}}—CH_3$$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Sp.Gr. 0.87. B.P. 201° C.

Practically insoluble in water, soluble in alcohol, Propylene glycol and oils.

Fruity, but also heavy-herbaceous, "incense-like" odor with mildly green-earthy, Reseda-like notes.

This ester of an alcohol which occurs in volatile oil of Coconut, finds a little use in perfumery for its peculiar Olibanum-Opopanax-Mignonette-type odor, blending well into modern fruity-green topnotes, e.g. the commonly used "Galbanum-plus-fruit-plus aldehyde" theme.

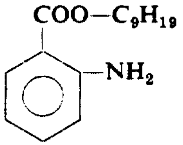
The ester is rarely offered commercially in the USA, and the author has no report of its possible use in flavors.

Prod.: by azeotropic esterification of *n-secondary*-Nonanol with Acetic acid.

163-57; 163-227;
See also: 103-201;

## 2365: NONYL ANTHRANILATE

*n*-Nonyl-*ortho*-aminobenzoate.
"Mandarinol N.A."
"N.A. ester".
Do not confuse with "Ether A.N." (Givaudan-Geneva) which is a different material.



$C_{16}H_{25}NO_2$ = 263.38

Colorless or pale straw-colored oily liquid. Sp.Gr. 1.03. B.P. 350° C.

Practically insoluble in water, soluble in alcohol and oils.

Very sweet, yet refreshingly "peel-like" Mandarin-Orange type odor with distinctly Orangeblossom-winey-fruity undertones and excellent tenacity.

Intensely sweet, Mandarin-Orange-like taste at concentrations near 1 ppm. This interesting ester is rarely offered in the USA, but has been used quite frequently in European perfumery and flavor compositions.

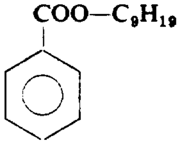
The ester offers pleasant variations in the Orangeblossom-theme with its unusual freshness and discretely green, peel-like notes. It blends particularly well with the equally rare *iso*-Butyl-*n*-methyl-anthranilate or similar esters, and it can be used in considerable amounts in Oriental fragrance types with Opopanax, Honey notes and Patchouli.

The ester is not listed as G.R.A.S. in the USA, but it may still be used in many other countries in Citrus flavors and "Tutti-frutti" types for hard candy, etc.

Prod.: from Isatoic anhydride and Nonyl-alcohol. This method will yield a colorless ester.

34-1011; 103-165; 163-228;

## 2366: NONYL BENZOATE



$C_{16}H_{24}O_2$ = 248.37

Colorless oily liquid. Sp.Gr. 0.96.
B.P. 315° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar, warm-herbaceous, sweet-fruity odor complex of considerable tenacity.

This ester, although rarely found in price lists, is occasionally used in perfume compositions, mainly of the "Oriental" and sweet-balsamic type with Ylang-Ylang, Opopanax, Myrrh, etc.

The material is missing in most perfume laboratories, and may be considered as practically obsolete in modern perfumery.

Prod.: by azeotropic esterification of *n*-Nonanol with Benzoic acid.

103-131; 163-228;

## 2367: NONYL-n-BUTYRATE

Nonyl butanoate.

$CH_3(CH_2)_8—OOC—CH_2—CH_2—CH_3$

$C_{13}H_{26}O_2 = 214.35$

Colorless liquid. Sp.Gr. 0.86. B.P. 228° C.

Very slightly soluble in water, soluble in alcohol and oils.

Heavy, sweet-fruity Orange-Rose, yet herbaceous odor of moderate tenacity.

This ester is very rarely found in commercial pricelists of perfume chemicals, but the *iso*-butyrate is occasionally found (see next monograph).

The title material could be used in modern versions of Oriental fragrance types, and in Lavender compositions with Opopanax and Clary Sage.

The author has no report of its possible use in flavor compositions, although some reports indicate that this – or the isomer – is used in flavors.

Prod.: by azeotropic esterification of *n*-Nonanol with *n*-Butyric acid.

140-139;

## 2368: NONYL-iso-BUTYRATE

*n*-Nonyl-*iso*-butanoate.

$CH_3(CH_2)_8—OOC—CH(CH_3)_2$

$C_{13}H_{26}O_2 = 214.35$

Colorless liquid. Sp.Gr. 0.86. B.P. 220° C.

Almost insoluble in water, soluble in alcohol and oils.

Delicately fruity, not as "deep" as the *n*-butyrate, yet a sweet-sharp Apricot-like, Orange-rosy, herbaceous-green odor of moderate tenacity.

This ester has found limited use in perfume compositions as a modifier in Oriental compositions with Galbanum, Patchouli, Lavender, Citrus oils, etc. The herbal-earthy-balsamic theme is not very interesting, and the ester is far from indispensable in modern perfumery. Many laboratories are perfectly happy without it.

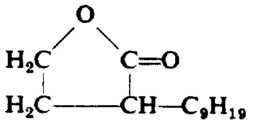
The ester has found use in flavor compositions for imitation Peach, Apricot, Orange and various fruit complexes in countries outside of the USA (where it is not considered G.R.A.S.).

Prod.: by azeotropic esterification of *n*-Nonanol with *iso*-Butyric acid.

33-734; 7-301; 103-116; 163-57;

## 2369: alpha-n-NONYL BUTYROLACTONE

Tridecanolide-*1*:*2*.
*alpha*-Nonyl-*gamma*-butyrolactone.



$C_{13}H_{24}O_2 = 212.34$

Almost colorless, oily, slightly viscous liquid. Sp.Gr. 0.92. B.P. 306° C.

Insoluble in water, soluble in alcohol and oils.

Floral, mildly Coconut-Peach-like odor with musky undertone and excellent tenacity.

This lactone, although of interesting odor type, has found very little, if any, use in perfumes or flavors. Its overall odor is rather weak, but its power should not be underestimated since it appears more conspicuously in combination with more volatile materials (lower esters, etc.).

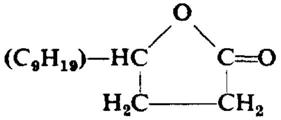
As an odor type, it ranks superior to the isomer (*gamma-n*-Nonyl-*gamma*-butyrolactone, see next monograph), but very few *alpha*-substituted *gamma*-lactones have found permanent use in perfumery or in flavors.

Prod.: from Nonylmalonic ester and Ethylene oxide.

31-170; 163-228; 156-229;

## 2370: gamma-n-**NONYL**-gamma-**BUTYROLACTONE**

Tridecanolide-*1*:*4*.
*gamma*-Tridecanolide.



$C_{13}H_{24}O_2 = 212.34$

Colorless, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Weak, fatty-grassy oily odor with mildly musky undertone and excellent tenacity.

This lactone is generally considered too weak to be of interest to the perfumer, and its odor type not sufficiently pleasant or versatile to encourage further experiments.

The *alpha*-substituted *gamma*-lactone is mentioned in the previous monograph, and it has had a little bit more success on account of its superior odor type, free from the grassy-fatty notes.

The material may be considered as practically obsolete.

Prod.:

1) from Nonyl ethylene oxide with Sodiomalonic ester.
2) by lactonization of *gamma*-Hydroxy tridecanoic acid.

31-170; 156-229;

## 2371: n-**NONYL CAPROATE**

Nonyl hexoate.
Nonyl hexylate.
Nonanol hexanoate.

$CH_3(CH_2)_8$—$OOC(CH_2)_4CH_3$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid. Sp.Gr. 0.89.
B.P. 255° C.

Insoluble in water, soluble in alcohol and oils.

Winey-ethereal, mildly fruity and nut-like odor of moderate tenacity.

Sweet, fruity-nut-like taste at concentrations below 20 ppm. The fruit notes are mostly Apple-like, while the nut-notes are Coconut-type.

This ester may have some use in perfumery, but the author is not aware of its use as a perfume material.

It has found some use in flavor compositions in countries other than the USA (where it is *not* listed as G.R.A.S.) for imitation Apple, Orange or Nut, usually in concentrations equal to 2 to 15 ppm in the finished product.

Prod.: by azeotropic esterification of *n*-Nonanol with Hexanoic acid.

34-1231; 103-181; 163-228;

## 2372: NONYL CAPRYLATE

*n*-Nonyl octoate.
Nonanol octanoate.
Nonyl octylate.

$CH_3(CH_2)_8{-}OOC(CH_2)_6CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 315° C.

Insoluble in water, soluble in alcohol and oils.

The existence of this ester in Bitter Orange oil has been known for several decades, but the material is rarely to be found in commercial pricelists.

Its peculiar sweet-rosy, delicately earthy-oily odor supplies a very attractive undertone in Orange flavor compositions, but it should be used with utmost discretion because of its unusual power as a flavor material.

The concentration normally applied is from 0.05 to 2 ppm in the finished consumer product. In other words, it will amount to one percent or less in an Orange oil flavor composition. Its taste is considerably improved in the presence of a mild food acid.

The "mushroomy" note in the title ester seems to be inherent to many derivatives of the C-9-family: Hexyl acrolein and *3*-Nonenol have more conspicuous, earthy-mushroomy notes at certain concentrations.

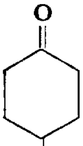
G.R.A.S. F.E.M.A. No.2790.

Prod.: by azeotropic esterification of *n*-Nonanol with *n*-Octanoic acid.

66-314; 90-92; 103-198; 163-228;

## 2373: para-NONYL CYCLOHEXANONE

*1*-Oxo-*4*-nonyl cyclohexane.
The commercial material consiststs mainly of the *para*-isomer.
The Nonyl-group consists of branched-chain isomers of alifatic Nonyl-. (See details in monograph: Nonyl phenol.).



$C_9H_{19}$ (branched-chain isomers).

$C_{15}H_{28}O = 224.39$

Colorless oily liquid. B.P. 262° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, but persistent woody-musky and soft-floral odor.

This ketone has been suggested for use in perfume compositions for its fixative effect and versatile woody-camphoraceous-musky character, blending well with Patchouli, Methylionones, Sandalwood, Cinnamic alcohol, Jasmin materials, etc. for woody or floral fragrance types.

Newer and more versatile, more well-defined chemicals were developed later than this prewar invention, and it seems most conceivable that the title material will never become a common perfume chemical. It was manufactured from a commercially available, industrial chemical which was very far from pure or well-defined.

Prod.: from Nonyl phenol by hydrogenation, followed by oxidation of the secondary alcohol to the title ketone.

31-99; French patent 850180(1939).

## 2374: NONYL FORMATE

*n*-Nonyl methanoate.
Nonanol formate.

$CH_3(CH_2)_8—OOC—H$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Refreshingly fruity-citrusy, sweet and lightly floral odor of moderate to poor tenacity.

Sweet citrusy, slightly waxy-fruity taste in concentrations near 20 ppm.

This ester has been used in perfume compositions for its interesting effect in Oriental fragrance types, particularly in combination with Olibanum. It is occasionally used in Chypre types or as part of a topnote complex for Rose, Orris and Oriental fragrances.

The title material is not listed as G.R.A.S. in the USA, but it has been suggested for use in imitation Apricot and Peach flavors in other countries.

Prod.: by azeotropic esterification of *n*-Nonanol with Formic acid.

103-85; 140-132; 163-57; 163-228;

## 2375: NONYL HEPTOATE

*n*-Nonyl heptanoate.
Nonanol heptylate.

$CH_3(CH_2)_8—OOC—(CH_2)_5CH_3$

$C_{16}H_{32}O_2 = 256.43$

Colorless liquid. Sp.Gr. 0.87. B.P. 300° C.

Insoluble in water, soluble in alcohol and oils.

Mildly green-herbaceous, sweet, Rose-Orangeblossom type odor of moderate tenacity.

This ester has been suggested for use in perfume compositions as a modifier in sweet floral and herbaceous-floral fragrance types, Chypre, Fougère, Orangeblossom, Oriental types, etc.

The ester is not much in use in the USA, but it is occasionally used in Europe in the more well-equipped perfume laboratories, although a perfumer can perfectly operate without this and many other Nonyl esters. These have, for some inexplicable reason, almost escaped the honorable life on a working perfumer's shelf.

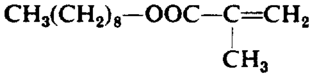
The author has no report of this ester being used in flavor compositions.

Prod.: by azeotropic esterification of *n*-Nonanol with Heptanoic acid.

35-61; 103-190; 163-57; 163-228;

## 2376: NONYL METHACRYLATE

Nonanol-*2*-methyl propenoate.
Nonanol-*alpha*-methylacrylate.



$$CH_3(CH_2)_8—OOC—\underset{\displaystyle CH_3}{\underset{|}{C}}{=}CH_2$$

$C_{13}H_{24}O_2 = 212.24$

Colorless oily liquid.
B.P. 232° C.

Insoluble in water, soluble in alcohol and oils.

Pungent-herbaceous-ethereal, but sweet and warm odor of moderate to poor tenacity.

This ester, developed in a range of esters for entirely different purpose (plastic and plexiglass) has been suggested for use in perfume compositions for its powerful lift and warm, ethereal character, blending excellently with Geranium, Lavender, Spike Lavender, etc. for detergent perfumes and similar type fragrances.

Although the ester is marketed with inhibitor which secures reasonable stability against polymerization, it seems most likely that the mere possibility of polymerization (which turns the ester odorless) has been sufficient reason for the perfumers to ignore the material.

It can be considered as practically obsolete as a perfume chemical today.

Prod.: by ester exchange reaction from Nonyl acetate and Methyl methacrylate. The methacrylates are unstable at elevated temperatures.

(Sample: Imperial Chemical Industries, Ltd.).

## 2377: NONYL PELARGONATE

Nonanol nonanoate.
*n*-Nonyl-*n*-nonylate.

$CH_3(CH_2)_8—OOC(CH_2)_7CH_3$

$C_{18}H_{36}O_2 = 284.49$

Colorless, slightly viscous liquid. Sp.Gr. 0.87. B.P. 315° C.

Insoluble in water, soluble in alcohol and oils.

Mild-fruity, oily-Orange-like odor of "aldehydic" character, but overall weak (mild).

The taste is relatively powerful – considering the apparent weakness of odor (probably due to the high boiling point), but the flavor is not very pleasant unless concentrations are kept as low as 1 to 5 ppm. Beyond that, the flavor is fatty more than fruity, waxy more than Orange-like.

The title ester has been suggested for use in perfume compositions. It is occasionally used in Oriental blends, or as part of the fixative base in Citrus colognes, Lavender bases, etc.

The material is rarely offered commercially and may become obsolete in perfumery within the next decade or so.

Prod.: by azeotropic esterification of *n*-Nonanol with *n*-Nonanoic acid.

103-205; 163-57; 163-228;

## 2378: NONYL PROPIONATE

*n*-Nonanol propanoate.

$CH_3(CH_2)_8—OOC—CH_2—CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Sp.Gr. 0.88. B.P. 245° C.

Almost insoluble in water, soluble in alcohol and oils.

Winey-ethereal, sweet-rosy and mildly waxy-aldehydic odor of moderate tenacity.

This ester, like most of the other Nonyl-esters, finds only limited use in perfumery. Although the odor is quite powerful, its type confines the field of application to the Oriental, Citrus or Rose type fragrances, and the concentration will in most cases be very low.

The title material blends very well with the musky-aldehydic, winey topnote types, including Cognac oil, Ambrette seed, various acetoacetic esters, etc.

Prod.: by azeotropic esterification of *n*-Nonanol with Propionic acid.

33-622; 103-108; 163-228;

## 2379: NONYL-n-VALERATE

*n*-Nonanol-*n*-pentanoate.

$CH_3(CH_2)_8—OOC(CH_2)_3CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless liquid. Sp.Gr. 0.88. B.P. 275° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm-fruity, slightly musty-floral odor with some resemblance to Hazelnut. Moderate tenacity.

This ester has been suggested for use in

perfume compositions along with Oakmoss and Citrus oils. It contributes a pleasant oily-herbaceous sweetness, not unlike the odor of Hazelnut. With the conventional "rose alcohols" it will enhance the Rosy tone, and it may similarly enhance an Orange oil note with sweet undertones.

The ester is unfortunately not often commercially available, but is generally prepared by the interested user himself. Accordingly, it is rarely found in the perfume laboratory, and many perfumers have never seen it or used it.

The title material is not listed specifically as G.R.A.S. in the American F.E.M.A. list, but the *iso*-Valerate is listed, and the two esters are often listed as one, or, commercially they are confused. As a supporting note to fruit complexes and modifier in nut imitation flavors, the ester has interesting possibilities. In some countries, however, the *iso*-Valerate is preferred for this purpose.

Prod.: by azeotropic esterification of *n*-Nonanol with *n*-Valeric acid.

33-933; 163-57; 163-228;

## 2380: NONYL-iso-VALERATE

Nonanol-*iso*-pentanoate.
Nonyl-*iso*-valerianate.

$CH_3(CH_2)_8—OOC—CH_2—CH(CH_3)_2$

$C_{14}H_{28}O_2 = 228.38$

Colorless liquid. Sp.Gr. 0.88. B.P. 264° C.

Insoluble in water, soluble in alcohol and oils.

Heavy-fruity, Apple-and-Hazelnut-like odor with citrus-winey notes. Moderate tenacity.

Sweet, oily-fruity, warm and discretely floral taste in concentrations below 5 ppm.

This ester is used in flavor compositions as a modifier in imitation Apple (interesting for Sherbet Ice flavor), in Orange and Hazelnut flavors, and in Tobacco flavors. It lends a very natural earthy-oily sweetness to Nut compositions, and this effect should be considered in perfumery, too.

The author has no report of the ester being used in perfume compositions, although it is most likely that any perfumer, who has access to this ester, would be interested in trying it out.

Concentration in finished flavored products is normally as low as 0.5 to 2 ppm.

G.R.A.S. F.E.M.A. No.2791.

See also: Nonyl-*n*-valerate (previous monograph).

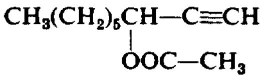
Prod.: by azeotropic esterification of *n*-Nonanol with *iso*-Valeric acid.

103-124;

## 2381: NONYNOL ACETATE

Noninol acetate.
The commercial product is an ill-defined mixture of isomers.

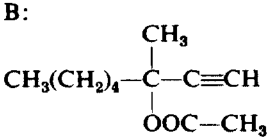
A:



$$CH_3(CH_2)_5\underset{\substack{|\\ OOC-CH_3}}{CH}-C\equiv CH$$

*2*-Nonyn-*3*-ol acetate.

B:



$$CH_3(CH_2)_4-\overset{\substack{CH_3\\ |}}{\underset{\substack{|\\ OOC-CH_3}}{C}}-C\equiv CH$$

*3*-Methyl-*1*-octyn-*3*-ol acetate.

$C_{11}H_{18}O_2 = 186.27$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-green, diffusive odor of moderate to poor tenacity. Various specialties of widely different composition and odor have been available of above or related identity.

The material has been suggested for use in perfume compositions for its refreshing, green-herbaceous and diffusive odor. The type is quite different from the Hexenyl-series, and offers much more versatility for use in floral fragrance types, e.g. Jasmin.

Prod.: various methods yield Nonynols:

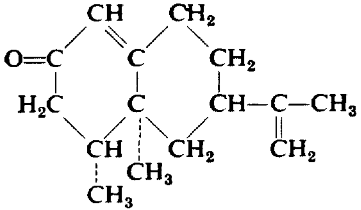
A: condensation of Heptaldehyde and Acetylene yields *2*-Nonyn-*3*-ol.

B: condensation of Methyl amyl ketone with Acetylene yields *3*-Methyl-*1*-octyn-*3*-ol.

Other methods are known and may afford different isomers. Acetylation will produce the ester.

## 2382: NOOTKATONE

*5,6*-Dimethyl-*8*-*iso*-propenylbicyclo-(*4,4,0*)-dec-*1*-en-*3*-one.



$C_{15}H_{22}O = 218.34$

Almost colorless, or pale yellowish oily liquid when pure. Some commercial grades are orange-colored, slightly viscous.

Practically insoluble in water, soluble in alcohol and oils.

This bicyclic, conjugated sesquiterpene ketone is relatively new even in the research laboratory. It was identified in Grapefruit peel oil and juice in the early 1960's and shortly after this discovery, a method of synthesis was developed, based upon a component of sweet Orange juice oil, Valencene.

The title material has an extremely powerful fruity, sweet and citrusy odor of good tenacity. The odor and flavor are very typical of Grapefruit peel oil in which the material may be present at the rate of about 0.3%.

Nootkatone has a pleasant taste in concentrations lower than 50 ppm, and although preliminary reports indicate that the material has a perceptible flavor down to 1 ppm, the author is inclined to claim that the minimum perceptible for Nootkatone is between 0.1 and 0.2 ppm. This is of course of minor importance. The interesting fact is that the material has a typical Grapefruit peel taste at levels higher than 3 ppm and lower than 50 ppm.

Nootkatone has been approved as G.R.A.S. by the American Food and Drug Administration, and it has been used very successfully in new carbonated beverages, etc. A highly purified synthetic product is now generally used.

The title ketone could undoubtedly find use in perfume compositions for novel effects in topntoe compositions, etc., particularly in combination with Bergamot oil, Bitter Orange oil, Hexenyl esters, Aldehydes, etc.

G.R.A.S. (FDA 1968).

Prod.: The sesquiterpene Valencene is isolated from Orange *juice* oil (a plentiful by-product) and oxidized with *tertiary*-Butyl chromate to yield the title ketone.

Samples: courtesy of Minute Maid Corporation, Plymouth, Florida, U.S.A.

Literature:

Journal of Food Science: 1964, vol. 29 (5), pages 565-568.

Journal of Food Science: 1965, vol. 30, page 876.

Tetrahedron letters, 1965, 4779.

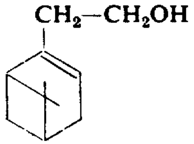
Ian Heilbron: Organic Chemical Comp. suppl. vol. 1966, page 151.

See also: 158-128.

Note: The title ketone should not be confused with Nootkatin, which is a ketone of entirely different odor type and structure, although its empirical formula is $C_{15}H_{20}O_2$.

## 2383: NOPOL

*6,6*-Dimethylbicyclo-(*3,1,1*)-*2*-heptene-*2*-ethanol.



$C_{11}H_{18}O = 166.27$

Colorless, slightly viscous liquid. Sp.Gr. 0.97. B.P. 220° C.

Very slightly soluble in water, soluble in alcohol and oils.

The material isomerizes if heated to its boiling point at atmospheric pressure.

Very mild, woody-camphoraceous odor of moderate to poor tenacity.

This alcohol was introduced about two decades ago and was initially thought to become a modifier for Terpineol. However, it does not have the floral tone or the versatility of Terpineol, even though the title material is available in a much higher state of chemical purity than the commercial Terpineol.

Nopol is by and large confined to woody and piney fragrance types, in which it may be the chief ingredient or "carrier". But its own odor contribution is very limited, and the title material will ruin almost any floral note if the Nopol is used at higher levels of concentration.

The esters of Nopol have become more popular and are used more widely (see next).

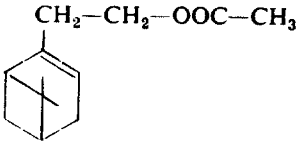
Prod.: by condensation of *beta*-Pinene with Formaldehyde under pressure (= at elevated temperature). Paraformaldehyde is often used in place of Formaldehyde.

(Glidden Co., data sheet May 1961).

87-175; 156-377; 163-228; 163-366;

## 2384: NOPYL ACETATE

"Citroviol" (Dow Chem. Co.).
"Lignyl acetate" (Shulton, Inc.).
*6,6*-Dimethylbicyclo-(*3,1,1*)-*2*-heptene-*2*-ethylacetate.



$C_{13}H_{20}O_2 = 208.30$

Colorless liquid. Sp.Gr. 0.98. B.P. 234° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, woody-fruity odor of moderate tenacity. Some similarity to Linalylacetate, however, less sweet, less fruity, more woody. A refined grade of Nopyl acetate shows more sweetness, less woody-piney odor.

This ester was introduced in the years of shortage and high prices of Linalyl acetate, and it had a considerable mission to fill at that time. Although it is no longer considered as a "substitute for Linalylacetate" it has found its place in perfumery as a versatile and low-cost sweet and fruity ester for use in Citrus, Fougère, Bergamot, Neroli, Cologne and soap perfumes, fragrances for various household products, etc. For many purposes, it gives better results than Terpinyl acetate and it is only slightly more expensive.

A few higher esters have been produced and made commercially available, but they have only minor importance in perfumery (see following monographs).

Prod.: by Acetylation of Nopol.

156-377; 163-228; 163-366;

## 2385: NOPYL-n-BUTYRATE

For full chemical name and structure, see: Nopol and Nopyl acetate.

$C_{11}H_{17}—OOC—C_3H_7$

$C_{15}H_{24}O_2 = 236.36$

Colorless oily liquid. Sp.Gr. 0.96.
B.P. 258° C.

Insoluble in water, soluble in alcohol and oils.

Sweet, but rather heavy, warm-herbaceous, almost spicy-balsamic odor of moderate tenacity.

This ester, rarely offered commercially, is occasionally used in perfume compositions as a supporting note for Clary Sage, Rosemary, Spike Lavender and other warm-herbaceous notes.

It performs well with Cinnamic alcohol and cinnamates in Chypre or woody-musky fragrance types, but it must be absolutely free from acid in order to perform in an attractive manner.

Prod.: from Nopol and *n*-Butyric anhydride.

156-377;

## 2386: NOPYL PROPIONATE

For full chemical name and structure, see: Nopol and Nopyl acetate.

$C_{11}H_{17}—OOC—C_2H_5$

$C_{14}H_{22}O_2 = 222.33$

Colorless liquid. Sp.Gr. 0.97. B.P. 245° C.

Insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, mildly spicy odor of moderate tenacity.

This ester finds some use in perfume compositions, e.g. as a modifier for Terpinyl propionate in low-cost Lavender types for detergents, household products, etc.

The odor is almost free from any trace of piney note, and quite large proportions can be used in ordinary compositions. The price of this ester is almost equal to that of Terpinyl propionate. It performs well with all common Ionones and Methylionones, and it gives pleasant variations in novel type Pine needle odors.

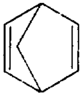
The material is commercially available.

Prod.: from Nopol and Propionic anhydride.

156-377;

## 2387: NOR-BORNADIENE

Bicyclo-(*2,2,1*)-hepta-*2,5*-diene.



$C_7H_8 = 92.14$

Colorless mobile liquid.

Insoluble in water, soluble in undiluted alcohol and oils, poorly soluble in diluted alcohol.

Very diffusive, gassy-piney, camphoraceous-woody odor (poor tenacity).

This hydrocarbon is industrially available as a chemical intermediate. It was not intended for use in perfumes, and it is only occasionally used as such. It serves mainly as a starting material for the manufacture of industrial chemicals, etc.

The material has occasionally been used in Pine needle fragrances to improve the diffusiveness of the fragrance, and to lend initial power and short life to the fragrances which are intended for "short-effect" purposes, e.g. dishwashing detergent fragrances, etc.

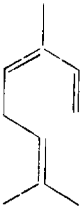
It is also used as a masking agent when a volatile and powerful material is needed at low cost.

Prod.: from Cyclopentadiene and Acetylene in a Diels-Alder type reaction.

(Sample: Shell Co. Chemicals Division).

## 2388: OCIMENE

The pure and desirable isomer is:
*3,7*-Dimethyl-*1,3,6*-octatriene.
Commercial grade Ocimene contains various amounts of several different isomers.
Allo-ocimene is a different material, see that monograph.



$C_{10}H_{16} = 136.24$

Colorless or very pale straw-colored mobile liquid. Sp.Gr. 0.80. B.P. 177° C.

Insoluble in water, soluble in alcohol and oils, poorly soluble in diluted alcohol, almost insoluble in Propylene glycol.

The material polymerizes easily and quickly when exposed to air (oxygen). Under Nitrogen or $CO_2$ it keeps well in storage.

Warm-herbaceous, very diffusive odor of poor tenacity. The sweetness is almost floral, and there is an immediate similarity to Neroli oil in the odor of pure Ocimene.

This terpene has recently become available in a very attractive state of purity. In that quality, Ocimene is a highly versatile perfume chemical, no longer just a masking agent

Pure Ocimene finds use in numerous artificial essential oils, Bergamot, Lavandin, Neroli, Orange, Basil, etc. etc., but it is also in itself an interesting material for new and powerful topnote effect in Citrus colognes, Lavender fougères, etc.

There is a very considerable difference in price between ordinary grade Ocimene and pure Ocimene, but the terpene is often used so sparingly that its relatively high cost is compensated for.

Commercial grade Ocimene is used as a starting material for the manufacture of a number of perfume chemicals, and it is also used occasionally as a perfume material for low-cost household-product fragrances, etc. It gives very pleasant effects with Bay oil in modern spicy-herbaceous fragrances.

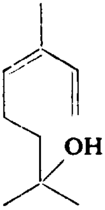
Prod.:

1) by thermal rearrangement of Pinene (type of pyrolysis).
2) Ocimene can also be prepared from Linalool.

31-5; 87-36; 100-740; 160-1126; 163-366;

## 2389: OCIMENOL

*2,6*-Dimethyl-*5,7*-octadien-*2*-ol.
or: *2,6*-Dimethyl-*3,5*-octadien-*2*-ol.



Exists in *cis*- and *trans*-forms. The *cis*-isomer is the preferred perfume material.

$C_{10}H_{18}O = 154.25$

Colorless oily liquid. B.P. 196° C.

Almost insoluble in water, soluble in alcohol and oils.

The material shows tendency of increasing its viscosity, but it maintains its odor for a much longer period than Myrcenol.

Diffusive and refreshing camphoraceous-Lime-like odor with an undertone of floral sweetness and – in spite of its low boiling point – a moderate to good tenacity.

This alcohol has only been commercially available since the early 1960's, and it has found its way into numerous fragrance types. Its "timing" was exceptionally good, since the increasing demand for Lime-type fragrances came after the mid-1960's, and the perfumer had very few chemicals on his shelf to provide him with a Lime-like odor of reasonable stability.

But the title material gives much more interesting results in floral and green-floral fragrance types, Muguet, Lily, Narcisse, etc. and in modern soap perfumes blending pleasantly with Lilial, Lyral, Cyclamal, Hydroxycitronellal, etc.

For the revived modern citrus-type cologne fragrance this material offers new tonalities, freshness and rich, cool notes, unobtainable with the natural Citrus oils.

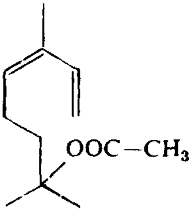
Prod.: from Ocimene by hydration, e.g. by Bertram-Walbaum's method (glacial Acetic acid and Sulfuric acid). The relatively poor yield is mainly responsible for the high cost of Ocimenol as compared to the inexpensive basic starting material (Pinene).

Ocimene may be obtained from Myrcene.

87-38;
See also: *3*,*7*-Dimethyl-*1*,*6*-octadien-*3*-ol.

## 2390: cis-OCIMENYL ACETATE

*2*,*6*-Dimethyl-*5*,*7*-octadien-*2*-yl acetate.
Commercial grade is mainly *cis*-isomer, which is the olfactorily preferred grade. The *trans*-isomer has a more pungent, weedy-harsh, Cuminyl-type odor.



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and refreshing, herbaceous-citrusy odor of moderate to poor tenacity.

This ester was only recently made commercially available and almost immediately found a place in artificial essential oils, Lavandin, Bergamot, etc.

Its fruity notes resemble the odor of Bartlett pear (preserved) and the material shows great versatility in use. As a modifier for all types of herbaceous fragrances, including Clary Sage, and in combination with Oakmoss and Styrax it gives new and attractive tonalities and pleasant freshness. It blends equally well with Labdanum products, Phenylethyl esters, Citronellol and esters, etc.

The title material could undoubtedly find use in flavor compositions if it were made permissible. It is *not* listed in the American G.R.A.S. list yet (Sept. 1968).

Prod.: by Acetylation of Ocimenol. The process is not very simple and the yield of acceptable material rather poor. Accordingly, the ester is relatively expensive.

(I.F.& F. sample).

## 2391: OCTADECANAL

Stearic aldehyde.
Stearaldehyde.
True "aldehyde C-18".

$CH_3(CH_2)_{16}CHO$

$C_{18}H_{36}O = 268.49$

Colorless or white, leafy crystals, or waxy, white mass. M.P. 38° C. B.P. 315° C.

Insoluble in water, fairly soluble in alcohol soluble in most oils.

Very faint, waxy, tenacious odor. Pure material is free from any trace of harsh or rancid notes.

The title aldehyde has been suggested for use in artificial flower absolutes, in Orris bases, etc.

The material is also mentioned here because of occasional confusion with the “so-called Aldehyde C-18”, which is included in this work under its chemical name: Nonanolide-*1,4*.

The two materials are in no way related to each other, and there is not even a similarity in chemical Nature or structure.

The author finds that the title material has little, if any, effect at all other than diluting a composition, and that the perfumer has many and better materials on hand to produce waxy flower notes, Orris notes, etc.

Prod.:
1) from Stearic acid via Stearyl alcohol by oxidation to the title aldehyde.
2) by reduction of Stearic acid, e. g. via its chloride.

Stearyl alcohol is listed in this work under the title: Octadecanol.

Stearic acid is listed in this work under the title: Stearic acid.

26-676; 31-37; 66-477; 159-408; 159-411; 160-1224; B-I-718;

## 2392: OCTADECANOL-1

*n*-Octadecyl alcohol.
Stenol.
Alcohol C-18.
“Lorol No. 28” (commercial grade, mainly Alcohol C-18).

$CH_3(CH_2)_{16}CH_2OH$

$C_{18}H_{38}O = 270.50$

Leafy colorless crystals or white crystalline mass. M.P. 60° C. B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Virtually odorless when pure, but commercial grades normally have a faint, bland-oily odor.

The title alcohol is used in cosmetic preparations at levels many times higher than the normal perfume level, and it is therefore interesting for the perfumer to know that this alcohol may act as a fixative and also as an odor-depressant upon the perfume or part of it.

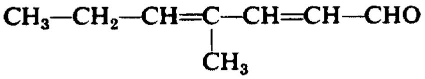
Furthermore, the odor of allegedly odorless materials should be tested by the perfumer prior to purchase or use, since trace impurities may include odors which are very difficult to combat. Off-odors in cosmetic raw materials are among the most common and troublesome problems to the working perfumer.

Prod.: from Stearic acid, which may be obtained by saponification of Tallow, or hydrogenation of Cottonseed oil, from Castor oil or from other natural oils.

26-640; 100-977; 160-1128; B-I-431;

## 2393: OCTADIENAL

Penteny1 acrolein.
*4*-Methyl-*2,4*-heptadien-*1*-al.



$$CH_3{-}CH_2{-}CH{=}\underset{\displaystyle CH_3}{\underset{|}{C}}{-}CH{=}CH{-}CHO$$

$C_8H_{12}O = 124.18$

Colorless or very pale yellowish oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and penetrating green-vegetable, grassy and somewhat fatty odor of moderate to poor tenacity.

This aldehyde, very rarely available, has been suggested for use in “green” bases, e.g. Galbanum compositions. In the years of shortage and exceptionally high prices of Galbanum (1964-65) there was a strong demand for chemicals supplying a Galbanum-like odor. Very few materials qualify for this type of fragrance.

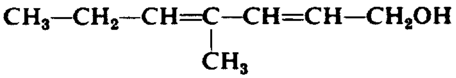
The author is of the impression that the title material is practically obsolete or at least not commercially available.

Prod.: by self-condensation of Propionaldehyde and subsequent condensation of the resulting *2*-Methyl-*2*-pentenal with Acetaldehyde to yield the title diolefinic aldehyde.

28-556;

## 2394: OCTADIENOL

*4*-Methyl-*2,4*-heptadien-*1*-ol.
Methyl butenyl propenol.



$CH_3{-}CH_2{-}CH{=}\underset{CH_3}{\underset{|}{C}}{-}CH{=}CH{-}CH_2OH$

$C_8H_{14}O = 126.20$

Colorless or very pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and very diffusive, sweet-oily, almost creamy-buttery, yet green and vegetable-like odor of moderate to poor tenacity.

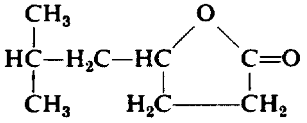
This alcohol has been suggested for use in perfume compositions, and it could undoubtedly produce interesting nuances – if applied with utmost discretion and experience – in many topnote compositions including Citrus, floral, "aldehydic", etc. It blends very well with Ylang-Ylang and the Methylionones, and supplies attractive notes to Mandarin, Coriander and other topnote materials.

However, the author is under the impression that the title material is no longer available, or it may be obsolete on account of production difficulties.

28-556;

## 2395: gamma-iso-**OCTALACTONE**

*iso*-Octanolide (*1*:*4*).
*gamma-iso*-Butyl-*gamma*-butyrolactone.
*iso*-Octyllactone.



$C_8H_{14}O_2 = 142.20$

Colorless oily liquid. B.P. 223° C.
Sp.Gr. 0.97.

Almost insoluble in water, soluble in alcohol and oils.

Powerful Coconut-coumarinic odor with herbaceous-spicy, almost Caraway-like and warm notes. Slightly greener, but less fatty than the *n*-Butyl butyrolactone, also more Caraway-like. Moderate tenacity. It does not have the tenacity of Coumarin, but it introduces the olfactory effect "higher" in the fragrance, and may therefore be used as an extender for Coumarin-like effects into the topnote of a fragrance.

Very sweet, Coconut-like, creamy-herbaceous and warm taste in concentrations near 5 ppm. Slightly bitter at concentrations higher than 50 ppm. Perceptible well below 1 ppm.

This lactone is used occasionally in perfume compositions as a modifier for Coumarin, and as a sweetener in heavy floral fragrance types, e.g. Gardenia. It gives interesting effects with Opopanax in Lavender compositions, and in Chypre, Fougère, Ambre and Oriental types with Tolu, Peru, Ylang-Ylang, Civet, Ionones, etc.

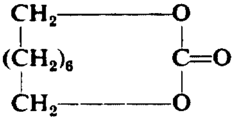
If the title material could be classified as G.R.A.S. in the USA, it could undoubtedly find many uses in flavor compositions, for Butterscotch, Caramel, Vanilla, Coconut, Hazelnut, etc. etc. The recommended concentration would then be about 5 to 20 ppm in the finished product.

Prod.: from *iso*-Butyl ethylene oxide plus Sodiomalonic ester.

See 416 = *alpha-n*-Butyl-*gamma*-butyrolactone.
(See also monograph: Octanolide-*1,4*) (2403).

## 2396: OCTAMETHYLENE CARBOXYLATE

Octamethylene carbonate.



$C_9H_{16}O_3 = 172.23$

Colorless viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Minty-musty, camphoraceous odor of moderate tenacity.

This material has been suggested for use in perfume compositions, mainly in soap perfumes with Patchouli and Spike Lavender oils, with which the title material blends well and gives lift and power to.

There are, however, many materials of this (or better) odor type with more power and versatility, and of better availability, wherefore it is reasonably safe to assume that the title material is or will soon be obsolete in perfumery.

Prod.: from Octamethylene glycol plus Diethylcarbonate by cross-esterification in presence of a Sodium catalyst. The resulting polymer is subsequently depolymerized, and the undesirable alcohol-surplus removed by boration.

30-272; 31-127; 159-439; 163-184;

## 2397: n-OCTANAL

Octyl aldehyde.
Octanal-*1*.
Caprylic aldehyde.
Aldehyde C-8.
*n*-Octaldehyde.
"Orange aldehyde" (old and confusing name).

$CH_3(CH_2)_6CHO$

$C_8H_{16}O = 128.22$

Colorless liquid. Sp.Gr. 0.80. B.P. 170° C.

Slightly soluble in water, soluble in alcohol and Propylene glycol under slowly progressive acetal-formation; soluble in oils.

Powerful, and in undiluted state harsh-fatty, penetrating odor. In extreme dilution sweet, Orange-like, slightly fatty, Honey-like and of moderate to poor tenacity. Oxidation to Caprylic acid takes place on a perfume blotter within 24 hours, and the acid odor will influence the odor picture over a prolonged period.

The taste in extreme dilution is sweet, fruity, Apricot-Plum-like, but becomes fatty, rather unpleasant at concentrations higher than 10 ppm.

This aldehyde is used in perfumery – always in minute concentrations – mainly as part of Rose topnotes, Neroli, Bergamot, Orange-blossom and in Citrus colognes, occasionally in Jasmin, etc.

It is also used extensively, but very sparingly, in flavor compositions for imitation Butter, Butterscotch, Chocolate, Apricot, Plum, Lemon-Orange, Cheese, Orange, etc. and in spice and condiment blends, e.g. Coriander, Celery, etc.

Concentrations are normally very low, e.g. 0.1 to 5 ppm in the finished product.

Prod.: (several methods) e.g. from Coconut fatty acids via Methyl-*n*-octoate or by catalytic oxidation of *n*-Octanol.

G.R.A.S. F.E.M.A. No.2797.

5-75; 31-48; 31-55; 41-30; 44-806; 26-450; 45-402; 66-477; 89-23; 84-3; 100-205; 106-33; 140-158; 156-18; 160-902; 163-58; 163-228; B-I-704.

## 2398: OCTANAL DIETHYLACETAL

*1,1*-Diethoxy octane.
Aldehyde C-8, diethylacetal.
Octylaldehyde diethylacetal.

$CH_3(CH_2)_6CH(OC_2H_5)_2$

$C_{12}H_{26}O_2 = 202.34$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

When absolutely free from aldehyde, this material has a pleasant sweet-woody, green and mildly floral odor, often including a winey or ethereal topnote.

This acetal has been suggested for use in perfume compositions as a modifier for woody-floral ingredients in Lilac, Muguet, etc. or as part of the fresh topnote where Cognac oil or similar ingredients are used.

The title acetal is rarely offered commercially.

Prod.:

1) from Ethyl alcohol and Octaldehyde by condensation.
2) from Heptylmagnesium bromide and Ethyl orthoformate.

163-58;

## 2399: OCTANAL DIMETHYLACETAL

*1,1*-Dimethoxy octane.
Aldehyde C-8, dimethylacetal.
Octaldehyde dimethylacetal.

$CH_3(CH_2)_6CH(OCH_3)_2$

$C_{10}H_{22}O_2 = 174.29$

Colorless liquid. Sp.Gr. 0.86. B.P. 185° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful oily-green and waxy-citrusy odor of poor tenacity.

The odor of the Dimethylacetal is not quite as interesting as that of the Diethylacetal. However, it seems that the Dimethylacetal is more freely available, more frequently used, and also favored with a place in the American G.R.A.S. list for food flavor chemicals.

The author is not aware of any extensive use of this Acetal in perfume compositions, although it could be used as part of a topnote complex for Citrus type colognes, or as part of an aldehydic-waxy complex for delicate floral bases.

The Acetal is used in flavor compositions for imitation Orange, Lemon, Melon, Coconut, in fruit complexes, Liqueur flavors, Cognac imitations, etc.

The normal concentration is about 0.5 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2798.

Prod.: by condensation of Octaldehyde with Methanol, e.g. using dry Hydrogen chloride gas as a dehydrating agent.

163-58; 163-228; 37-281;

## 2400: OCTANOIC ACID

Caprylic acid.
*n*-Octylic acid.
*n*-Octoic acid.
C-8 acid.
NOTE: *2*-Ethyl hexanoic acid is also called "Caprylic acid".

$CH_3(CH_2)_6COOH$

$C_8H_{16}O_2 = 144.17$

Colorless liquid, solidifying in the cold to a crystalline mass or leafy crystals melting at 17° C. Sp.Gr. 0.91 (liquid). B.P. 239° C.

Poorly soluble in cold water, 0.2% soluble in hot water, soluble in Propylene glycol, miscible with alcohol and oils.

Oily-rancid, sweat-like odor, repulsive to most people, even in dilution of less than 0.1% acid.

Alcoholic solutions will quickly acquire a pleasant fruity note of the Ethylester.

Burning, acid-acrid and rancid taste at concentrations higher than 50 ppm. Cheesy-sour at lower concentrations.

This acid finds very little use in perfumery, beyond that of traces in various artificial essential oils, imitation Civet, etc.

In flavor compositions, it is used for imitation Butter, Coconut, Cheese, Honey, Pineapple, Brandy, etc., usually at concentrations varying from 3 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2799.

Prod.: by isolation from Coconut fatty acids, via the esters to the alcohol.

*2*-Ethyl hexanoic acid is a petrochemical derivative.

26-450; 66-577; 90-88; 100-205; 140-142; 160-902; B-II-347; 163-184;

## 2401: OCTANOL-1

*1*-Octanol.
*n*-Octyl alcohol.
Alcohol C-8.
*n*-Caprylalcohol. (This name also used for *2*-Octanol).
Heptyl carbinol.

$CH_3(CH_2)_6CH_2OH$

$C_8H_{18}O = 130.23$

Colorless, slightly oily liquid. Sp.Gr. 0.83. B.P. 195° C.

0.05% soluble in water, soluble in Propylene glycol, miscible with alcohol and oils.

Powerful, fresh, Orange-Rose-like, waxy and sweet odor of poor tenacity. Balsamic-herbal undertones are often classified as Opopanax-like. Oily-fruity, sweet and slightly herbaceous taste at about 5 ppm.

This alcohol finds limited use in perfumery, although widely distributed in many types of fragrance: Rose, Jasmin, Sweet Pea, Honey, Orangeblossom, Citrus colognes, sophisticated Pine needle odors, waxy floral odors, etc.

It blends very well with Rose, Ylang-Ylang, Opopanax, Orange oil, Linalool, etc. and it is more powerful than the unexperienced perfumer will expect. Even amounts of less than one percent may demand skillful fixation in order to perform in an attractive way.

The title alcohol is used in trace amounts in imitation Peach, Pineapple, Coconut, Chocolate, and in various citrus and fruit complexes.

Concentration is normally about 1 to 3 ppm in the finished product, but may reach 15 to 60 ppm in chewing gum.

Prod.: from Coconut fatty acids, e.g. reduction of Methylcaprylate with Sodium ethoxide.

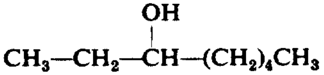
G.R.A.S. F.E.M.A. No.2800.

26-642; 29-476; 31-15; 34-806; 35-400; 35-402; 41-22; 84-2; 85-92; 100-743; 106-26; 140-124; 160-1130; 163-58; 163-228; B-I-418;

See also:
Methyl hexyl carbinol (Octanol-*2*). (2057).
*2*-Ethyl hexyl alcohol ("Octyl alcohol"). (1260).
*3*-Octanol. (2402).

## 2402: 3-OCTANOL

Ethyl-*n*-amyl carbinol.
*d*-*n*-Octanol.



$$CH_3{-}CH_2{-}\overset{\overset{\displaystyle OH}{|}}{C}H{-}(CH_2)_4CH_3$$

$C_8H_{18}O = 130.23$

Colorless liquid. Sp.Gr. 0.82. B.P. 179° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and powerfully herbaceous, oily-nutty and warm odor. Milder and not as harsh as that of *2*-Octanol, much warmer than *1*-Octanol. Moderate to poor tenacity.

This alcohol has found quite extensive use in perfume compositions, although always in low concentrations. Its main use is in artificial Spearmint, Lavender, Lavandin, Cornmint oils, etc. and in traces in Fougères, etc. along with Oakmoss. In less than 2%, often less than 1% concentration in the perfume oil, it introduces a warmth and deep herbaceous-oily note which is difficult to obtain with any other single material. Its low boiling point contributes to the difficulty in using higher concentrations, even under solid fixation of the fragrance.

The alcohol finds some use in flavor compositions, mainly as a trace ingredient in imitation Coconut.

G.R.A.S. (by F.E.M.A.).

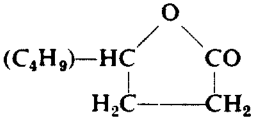
Prod.: by hydrogenation of Ethyl-*n*-amyl-ketone.

5-71; 5-149; 45-401; 45-402; 77-171; 87-471; 163-228;

See also monographs:
Octanol-*1*. (2401).
Methyl hexyl carbinol (= *2*-Octanol). (2057).
*2*-Ethyl hexylalcohol ("Octyl alcohol"). (1260).

## 2403: OCTANOLIDE-1,4

*n*-Octalactone.
*gamma*-Octalactone.
*gamma*-*n*-Butyl-*gamma*-butyrolactone.
Caprylolactone.
NOTE: *gamma*-iso-Octalactone is listed under that name. (2395).



$C_8H_{14}O_2 = 142.20$

Colorless slightly oily liquid. Sp.Gr. 0.98. B.P. 234° C.

Slightly soluble in water, soluble in alcohol and oils, fairly soluble in Propylene glycol.

Sweet-herbaceous Coconut-like odor with an oily Tonka-bean-like undertone.

Very sweet taste, reminiscent of Coconut and Tonkabean, with an herbaceous and pleasant aroma.

The odor of this chemical is described in various literature as "Caraway-like Cumin" (86-28) and (31-173) "Peach" (86-105) but the author disagrees strongly, assuming that a mistake must be responsible for those descriptions.

This lactone is used in perfumery in heavy floral fragrances such as Gardenia, Tuberose, Hyacinth, and even in Lily. It serves as an interesting modifier or substitute for Coumarin in herbaceous fragrance types, Fougères, Lavenders, etc. In spite of its comparatively low boiling point, it has an excellent tenacity.

Suggested for use in flavor compositions, where this lactone may form a base for Coconut, Nut, Butter-nut imitation flavors, and be a part of Vanilla compositions, Butter, Cheese, Caramel, Treacle, Rum, etc. A combination of 15% Octanolide plus 85% Cyclotene shows a Coumarin-like taste in concentrations near 2 ppm. The title material is normally used at 5 to 60 ppm in the finished product.

Prod.: from Epoxy-*1*,*2*-hexane plus Sodiomalonic ester. After saponification, the oxy-acid is extracted with ether and lactonized.

G.R.A.S. F.E.M.A. No.2796.

4-106; 31-173; 86-26; 106-282; 156-229;

## 2404: 3-OCTANON-1-OL

Hexanoyl ethanol.
Caproyl ethanol.
Methylol methyl amyl ketone.
"Ketone alcohol".
A *beta*-Ketol (or *1:3*-Ketol).

$CH_3(CH_2)_4CO—CH_2—CH_2OH$

$C_8H_{16}O_2 = 144.22$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, herbaceous-fruity, mildly spicy odor of moderate tenacity.

Warm-fruity-herbaceous, "condiment"-like taste in concentrations below 5 ppm. The taste tends to be slightly bitter at concentrations higher than 20 ppm.

This Ketol has found a little use in perfumery as a modifier in Lavender, Fougère, Spice, Rondeletia and other fragrance types, particularly for soap.

It is used in fruit and spice flavor blends at concentrations equal to about 0.2 to 1 ppm in the finished product. The author feels that the low concentration is more due to a disliking of the effect of the material than it is due to actual power of this Ketol.

Although not obsolete, this material can be classified as relatively dispensable in flavor creation.

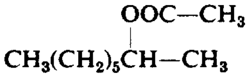
G.R.A.S. (by F.E.M.A.).

Prod.: by condensation of Methyl amyl ketone with Formaldehyde under mildly alkaline conditions.

See also: *3*-Nonanon-*1*-yl acetate.

## 2405: 2-OCTANYL ACETATE

Methyl hexyl carbinyl acetate.
Methyl-*n*-hexyl carbinyl acetate (correct name).
Commercial (industrial) Methyl hexyl carbinyl acetate is often Methyl-*iso*-hexyl carbinyl acetate, which is listed in this work under *2*-Methylheptanol-*6*-acetate.
The title name in this monograph has also been selected in order to reduce the confusion in the nomenclature of the *iso*-Octylacetates.



$$CH_3(CH_2)_5\overset{\overset{\displaystyle OOC—CH_3}{|}}{C}H—CH_3$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Sp.Gr. 0.87. B.P. 196° C.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-floral and herbaceous odorcomplex. The fruity notes being of Apple-citrus character, the floral-herbaceous notes resembling part of Jasmin, while the earthy-herbaceous undertones point in the Fougère direction. The author feels that the latter note may be due to traces of the unacetylated carbinol, while a pure ester would have an overall fresher odor, less complex.

This ester is occasionally used in perfumery, but it should be noted that much confusion exists in the nomenclature of "*secondary*"-Octyl alcohol. The title ester (and its parent carbinol) is however, the most common industrial isomer, and by far the least expensive.

Apart from scattered use in Lavender, Lavender-Rose, Chypre and in various types of soap fragrance, this ester is not a common item on the perfumer's shelf.

It finds some use in flavor compositions as a modifier in Citrus flavors, fruit complexes, Blackcurrant and other berry types, etc.

Prod.: by acetylation of Methyl hexyl carbinol.

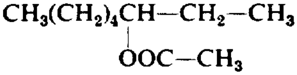
G.R.A.S. F.E.M.A. No.2806.

33-502; B-II-134;
See also: *3*-Octanyl acetate (next).

## 2406: 3-OCTANYL ACETATE

Ethyl-*n*-amyl carbinyl acetate.

**Note**: This material is often called "*secondary*"-Octyl acetate in perfumery literature, which may cause confusion with Methyl hexyl carbinyl acetate.



$$\begin{array}{l} CH_3(CH_2)_4CH-CH_2-CH_3 \\ \quad\quad\quad\quad\;\; | \\ \quad\quad\quad\quad\;\; OOC-CH_3 \end{array}$$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Sp.Gr. 0.86. B.P. 187° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Refreshing and rather delicate, rosy-minty odor of moderate to poor tenacity.

This ester has found some use in perfumery as a modifier in floral-herbaceous fragrance types, since it blends equally well with Lavender and Rose, with Opopanax and Geranium, etc. It is also used as a modifier in minty fragrance types to introduce freshness and mild, warm notes without the weedy-green notes often accompanying the Mint materials.

There is a considerable difference between the odor of this ester and the acetates of the isomer Octanols. Unfortunately, the title ester is one of the comparatively expensive Octanyl-acetates, and its use is therefore somewhat restricted.

It should not be confused with the acetate of Ethyl-*iso*-amyl carbinol which is an inexpensive, industrial petrochemical of entirely different odor type.

Prod.: by direct esterification of *3*-Octanol with Acetic acid or Acetic anhydride.

7-168; 28-607; 35-401; 163-228; 103-95; 90-211;

See also:
*2*-Octanyl acetate. (2405).
*n*-Octyl acetate. (2408).
*2*-Methylheptanol-*6*-acetate. (2041).
*2*-Ethyl hexyl acetate. (1262).
Ethyl-*iso*-amylcarbinylacetate. (1147).

## 2407: 2-OCTENOIC ACID

*n*-Pentyl acrylic acid.

$CH_3(CH_2)_4CH{=}CH{-}COOH$

$C_8H_{14}O_2 = 142.20$

Colorless liquid. Sp.Gr. 0.98. B.P. 228° C.

Almost insoluble in water, soluble in alcohol and oils.

Relatively powerful, oily-musty odor, in dilution more fruity and pleasant. Moderate to good tenacity, but unpleasant when undiluted.

This acid has found a little use in perfumery as a trace ingredient in artificial essential oils, etc.

It has been suggested for use in flavor compositions, but at this time (Oct. 1968) it has not yet been listed as G.R.A.S. by the American authorities. It could probably be used in imitation Cheese, Butter, Nut, Butterscotch compositions, etc.

Prod.:

1) from Hexaldehyde by the Döbner reaction.
2) by regulated hydrogenation of *2*-Octynoic acid.

6-638; 163-367;

## 2408: n-OCTYL ACETATE

Octanyl acetate.
Capryl acetate.
Acetate C-8.

**Note**: The title name is also used commercially for *2*-Ethyl hexyl acetate, see that monograph. (1262).

$CH_3(CH_2)_6CH_2{-}OOC{-}CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless liquid. Sp.Gr. 0.87. B.P. 208° C.

Very slightly soluble in water, soluble in alcohol and oils.

Fruity, slightly fatty, waxy-floral odor with a discretely green, Apple-like or almost "weedy" note, while the undertones are mildly woody. Moderate to poor tenacity.

This ester finds some use, although always at very low concentration, in perfume compositions, e.g. Jasmin, Gardenia, Orange-blossom, Citrus, Orris, etc. and in many fruity-woody types, Chypres, Fougères, etc. Traces may be used in Cassie, Neroli, Rose, Violet, etc. but the ester must be handled with discretion and supported by clever fixation in order to perform delicately and not "stand out" of the composition.

In flavors, minute amounts are used in imitation Raspberry, Apple, Cherry, Strawberry, Lemon, Peach, Pear, Brandy, etc. and in "tutti-frutti" complexes, etc.

The normal concentration of this ester in the finished product will be about 1 to 6 ppm.

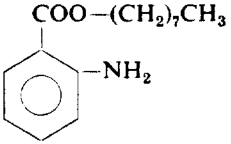
G.R.A.S. (by F.E.M.A.).

Prod.: by azeotropic esterification of *n*-Octanol with Acetic acid.

41-14; 33-501; 33-502; 31-122; 100-742; 106-17; 103-95; 163-58; 26-642; B-II-134;

## 2409: n-OCTYL ANTHRANILATE

*n*-Octyl-*2*-aminobenzoate.



$C_{15}H_{23}NO_2 = 249.36$

Colorless or very pale straw-colored oily liquid. Sp.Gr. 1.03. B.P. 320° C.

Insoluble in water, soluble in alcohol and oils.

Fresh-oily, herbaceous-floral and very sweet, tenacious odor of Sweet-Pea and Neroli-type, often compared to "Frangipanni" (or "Plumeria").

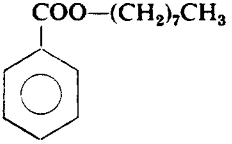
This ester has occasionally been available for perfumery use, but it does not seem to have enjoyed any strong demand.

The ester lacks character and it can hardly excite a perfumer with an average material library at hand. It is the type of material one might use if it were on the shelf, but one would not miss if it never arrived at the laboratory.

Prod.: from *n*-Octanol and Isatoic anhydride.

34-1011; 163-229;

## 2410: OCTYL BENZOATE



$C_{15}H_{22}O_2 = 234.34$

Colorless or very pale straw-colored, slightly viscous liquid. Sp.Gr. 0.97. B.P. 305° C.

Insoluble in water, soluble in alcohol and oils.

Rather weak, balsamic-oily odor of considerable tenacity.

Apart from occasional use as a fixative (of very low odor value), this ester may only find very infrequent use in Chypre, Fougère, Wood or Oriental fragrance types. Yet, it is definitely dispensable in such fragrances, and the perfumer will normally have a good number of other materials in mind for such projects.

The ester has been recommended for use in imitation Banana flavor, and it does, to some extent, supply the dull-juiceless, mildly oily taste or mouthfeel, which is typical of part of the Banana flavor picture. Traces of Mimosa absolute are of very interesting effect in such experiments.

Prod.: by azeotropic esterification of *n*-Octanol with Benzoic acid.

7-305; 163-58; 163-229; 35-404; 103-130;

## 2411: OCTYL-n-BUTYRATE

$CH_3(CH_2)_7—OOC(CH_2)_2CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. B.P. 244° C. Sp.Gr. 0.86.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar, green-herbaceous, remotely Orange-like and mildly fatty-floral odor. The herbaceous notes resemble the warmer parts of Galbanum, while the floral notes are related to Rose. Moderate tenacity.

This ester finds a little use in perfume compositions for Rose, Geranium, Chypre bases, Fougères, etc. and its power should not be underestimated since normal use concentration would be about 0.5 to 2% in the fragrance composition.

The ester has a pleasant, green-fruity taste in concentrations below 5 ppm, while it is rather harsh, oily-vegetable at higher levels.

It is used in many types of flavor, e. g. Butter, Citrus, Cucumber, Cherry, Melon, Liqueur flavors, Fruit complexes, Peach, Pistacio, Pineapple, Strawberry, etc.

The concentration in the finished product will normally be as low as 0.5 to 3 ppm.

G.R.A.S. F.E.M.A. No.2807.

Prod.: by azeotropic esterification of *n*-Octanol with *n*-Butyric acid or by conventional method from *n*-Butyric anhydride.

35-404; 90-214; 163-58; 163-229;

## 2412: OCTYL-iso-BUTYRATE

$CH_3(CH_2)_7—OOC—CH(CH_3)_2$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Sp.Gr. 0.87. B.P. 237° C.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing, herbaceous and fruity-green, vegetable odor. Some observers find it "crude", but this may be personal impression of a poorer grade material. The odor will inevitably call sweet memories to those who have grown up in the country, where the giant Bear's Claw is found, or it may smell "rooty" or "mushroomy" or "earthy" to others.

This material may tempt a perfumer to use it in Chypre, "tabac", Fougère, Lavender, New Mown Hay, "Bruyère" etc. in fact the typical "outdoor" odors. It gives very pleasant effects with Ethyl Chrysanthemumate and Labdanum products, Coumarin, Oakmoss, Galbanum, etc.

Its taste is a little less floral than that of the *n*-Butyrate, and perhaps more vegetable-herbaceous.

It is used in imitation Pistacio, Grape, Melon, Peach, Citrus complexes, fruit blends, wine and Liqueur flavors, ect.

The concentration is normally about 2 to 4 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2808.

Prod.: by azeotropic esterification of *n*-Octanol with *iso*-Butyric acid, or under ordinary conditions with *iso*-Butyric anhydride.

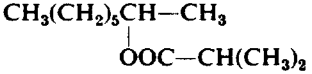
33-734; 35-404; 163-229;

## 2413: secondary-OCTYL-iso-BUTYRATE

*2*-Octanyl-*iso*-butyrate.

Methylhexylcarbinyl-*iso*-butyrate.

Note: Perfumery literature often uses the title name for Ethyl-*n*-amyl-carbinyl-*iso*-butyrate, which is *3*-Octanyl-*iso*-butyrate, an isomer. The author believes that the title material is the most common of the two isomers.



$$\begin{array}{l} CH_3(CH_2)_5CH—CH_3 \\ \qquad\qquad\;\; | \\ \qquad\qquad OOC—CH(CH_3)_2 \end{array}$$

$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. B.P. 232° C. Sp.Gr. 0.85.

Practically insoluble in water, soluble in alcohol and oils.

Fruity-rosy, floral and fresh odor of moderate to good tenacity. Fresher odor than that of the *n*-Butyrate. The fruity notes being light, Melon-Peach-like.

This ester finds very little use in perfume compositions, e. g. as a modifier for floral-fruity-herbaceous notes in Chypre or modern herbaceous-aldehydic fragrance types. It is rarely found in a perfume laboratory, and most perfumers probably never see or use it.

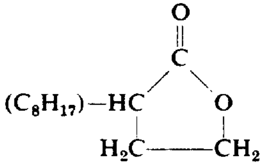
In flavors, it has been used for imitation Apricot, Peach and Melon, but not very commonly.

Prod.: by azeotropic esterification of 2-Octanol with *iso*-Butyric acid.

35-404; 163-59;

## **2414:** alpha-**OCTYL**-gamma-**BUTYROLACTONE**

Dodecanolide-*1:4*.
*alpha*-Dodecanolide.
A Dodecalactone, sometimes called *alpha*-Dodecalactone.



$C_{12}H_{22}O_2 = 198.31$

Colorless or very pale straw-colored, slightly viscous liquid. B.P. approximately 290° C (extrapolated), Sp.Gr. 0.94.

Practically insoluble in water, soluble in alcohol and oils.

Very tenacious, but delicately green-peachy odor with unquestionably musky undertones.

This lactone has been suggested for use in perfume compositions, and several specialties have been based upon this chemical. There are perfumers who prefer it over the conventional Undecalactone for "peachy" effect, partly because it is accompanied by musky undertones and partly because it carries a discretely refreshing, green note.

It blends very well with Oakmoss for bases in modern perfumes, and it gives excellent fixation when supported by Sandalwood, macrocyclic musks, Vetiver, etc.

The title material has not been mentioned in connection with flavors, and it is not listed specifically as G.R.A.S. in the American Federal Register or by the F.E.M.A. However, it could undoubtedly find use as a modifier in Peach and Apricot imitation, and as a fixative for heavy-fruity blends.

Its taste is sweet-fruity, Peach-like at concentrations below 5 ppm, and its minimum perceptible level is far below 1 ppm.

Prod.: from Octyl malonic ester and Ethylene oxide.

156-229; 163-229;

## **2415: OCTYL CAPROATE**

*n*-Octyl hexoate.
Octyl hexanoate.
Octyl hexylate.

$CH_3(CH_2)_7—OOC(CH_2)_4CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 275° C.

Insoluble in water, soluble in alcohol and oils.

Bland-fruity, also mildly herbaceous odor of considerable tenacity. The odor seems to lack character, and its initial power is very limited. Only in composition with more volatile materials it may show some effect, generally fruity, Banana-like and mildly green or almost "metallic" as Parsley.

This ester has been suggested for use in perfume compositions, but the author is under the impression that it is very rarely, if ever, used to any extent.

Prod.: by azeotropic esterification of *n*-Octanol with Caproic acid.

34-1230; 35-404; 90-215; 163-229;

## 2416: n-OCTYL CAPRYLATE

*n*-Octyl octoate.
Octyl octylate.
Octyl octanoate.

$CH_3(CH_2)_7{-}OOC(CH_2)_6CH_3$

$C_{16}H_{32}O_2 = 256.43$

Colorless oily liquid. B.P. 307° C.
Sp.Gr. 0.86.

Practically insoluble in water, soluble in alcohol and oils.

Weak, but persistent and sweet-herbaceous, almost tea-like odor. Esters containing one or the other parent chemical, alcohol or acid, show entirely different odor, usually unpleasant, fatty-oily, or even acrid. A perfectly balanced ester has a pleasant, but very mild or weak odor.

The taste in concentrations below 5 ppm is oily-fruity, sweet, mildly green or herbaceous. Higher concentrations tend to produce bitter-herbaceous and unnatural notes.

This ester has been suggested for use in perfume compositions, but the author finds that there is no important use of it, nor any demand for this ester in perfumery.

It finds limited use in flavor compositions, mainly in Citrus complexes, Cherry, Grape, Pineapple, Plum and other fruit imitation flavors.

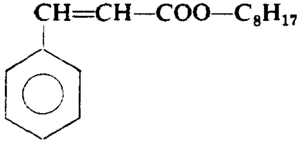
The concentration is normally about 0.5 to 2 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2811.

Prod. by azeotropic esterification of *n*-Octanol with Octanoic acid.

35-404; 90-217;

## 2417: OCTYL CINNAMATE



$C_{17}H_{24}O_2 = 260.38$

Colorless, slightly viscous liquid.
Sp.Gr. 0.96. B.P. higher than 320° C.

Insoluble in water, soluble in alcohol and oils.

Very mild, but sweet and tenacious, balsamic odor. The sweetness is more herbaceous-spicy than fruity, and it is often described as Opopanax-like.

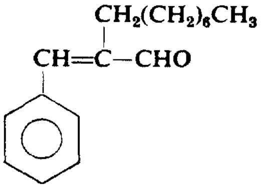
This ester has been suggested for use in perfume compositions, and it has occasionally been used in heavy Oriental fragrance types such as "Shamilar" types, where Castoreum, Opopanax and heavy-sweet wood odors are connected to rich, sweet florals with a strong emphasis upon balsamic fixative notes, also including Vanillin.

The title material also performs well with Oakmoss and Methylionones, and with *iso*-Eugenol in "l'Origan" modifications, etc.

Prod.: by azeotropic esterification of *n*-Octanol with Cinnamic acid. Also by alcohol interchange reaction with Methyl cinnamate.

34-462; 35-404; 163-229;

## 2418: alpha-n-OCTYL CINNAMIC ALDEHYDE



$C_{17}H_{24}O = 244.38$

Viscous yellowish oil. B.P. 289° C.
Sp.Gr. 0.93.

Insoluble in water, soluble in alcohol and oils.

When this material is absolutely pure, it is virtually odorless (in the opinion of most perfumers). Older odor descriptions seem to indicate that the material has been available in a rather impure state, with Benzaldehyde-notes more or less perceptible.

The material could find some use as a fixative/blender in Jasmin and Tuberose bases where the very mild oily-green odor of the subject material could be forced out in presence of larger amounts of more volatile components. However, in competition with the two favored members of the series, Amyl- and Hexyl-, the title material has really nothing to offer, and it is inevitably more expensive than the two others.

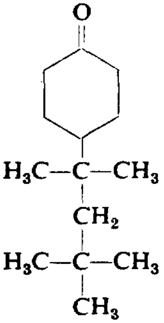
In view of the above, the author would consider the title material practically obsolete in perfumery.

Prod.: by condensation of Decylaldehyde with Benzaldehyde under mildly alkaline conditions.

31-51; 93-150;

## 2419: para-**OCTYL CYCLOHEXANONE**

*1*-Oxo-*4*-octylcyclohexane.
"Ordilon" (Norda).
- and other trade names.
The commercial material consists mainly of the *para*-isomer.
The Butyl-radicle consists mostly of branched-chain Octyl isomers and the structure below indicates the chief component:
*4*-(*2,2,4,4*-Tetramethylbutyl-)-cyclohexanone:



$C_{14}H_{26}O = 210.36$

Colorless liquid. B.P. 251° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, oily-woody, almost floral odor of considerable tenacity. The undiluted material may appear somewhat camphoraceous, but its effect is rather sweet and floral-woody in compositions.

This ketone – another old Bayer patent – is available as a perfume chemical among an extensive series of alkyl cyclohexanones.

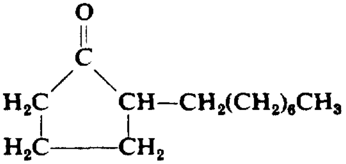
It finds use in soap perfumes with Methylionones, Phenylethyl alcohol, Sandela, Cinnamic alcohol and similar type materials.

It is very stable in soap and also stable against daylight or normal chemical exposure, but it is not a perfume chemical with a special character.

Prod.: from *para*-Octylphenol (an industrial chemical) by hydrogenation followed by oxidation of the secondary alcohol.

31-99; (Norda); French pat. 850180 (1939).
See monograph: Octyl phenol.
See also: Journal of American Chemical Society 1948, vol. 70, page 1474.

## 2420: alpha-**OCTYL CYCLOPENTANONE**



$C_{13}H_{24}O = 196.34$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and oily-floral, mildly balsamic-herbaceous odor of excellent tenacity.

This ketone has been suggested for use in perfumes and as a modifier for the lower homologues, many of which have Jasmine-type of odor.

The title material has been incorporated in specialties, but the author is of the impression that it is no longer commonly used in perfumes.

Prod.: by condensation of Octylaldehyde and Cyclopentanone, followed by hydrogenation of the unsaturated condensation product.

French patent No. 779789 (by L.Givaudan 1935).

31-86;

## 2421: OCTYLENE

*1*-Octene.
Caprylene.
*alpha*-Octylene.
The title material is one of many known isomers of this Olefin.

$CH_3(CH_2)_5CH{=}CH_2$

$C_8H_{16} = 112.22$

Colorless mobile liquid. Sp.Gr. 0.72.
B.P. 123° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Sweet-ethereal, diffusive odor. It is characteristic of the (higher) Olefins that they do not display the "gassy" pungency of the Acetylenes, nor the "gasoline-ethereal" odor of the Paraffins of same number of Carbon atoms.

This material serves mainly as an intermediate in the manufacture of other perfume chemicals, but is has occasionally been used in industrial masking odors, etc. on account of its volatility and sweet odor.

Prod.:
1) from Allyl chloride and *n*-Amyl magnesium bromide.
2) from Octanol with Iodine and red Phosphorous.
3) from Monosodium acetylene with Octyl iodide in liquid Ammonia at 40° C. under pressure.

1-55; 26-644; 100-205; 160-1132; B-I-221; Comptes Rendus 168-825;

## 2422: n-OCTYL FORMATE

Octyl methanoate.

$CH_3(CH_2)_7OOC{-}H$

$C_9H_{18}O_2 = 158.24$

Colorless mobile liquid. B.P. 200° C.
Sp.Gr. 0.87.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and relatively diffusive, fruity-green, Orris-Rose type odor of poor tenacity.

Refreshing, fruity-green taste in concentrations below 10 ppm.

This ester finds a little use in perfume compositions as a modifier in Orris compositions, Rose bases, Orange types, etc. It is often used with Palmarosa oil to introduce a natural freshness to that material.

In flavors, the ester finds its way into "tutti-frutti" compositions, Peach and Apricot imitations and various Citrus types. The concentration is normally about 0.5 to 8 ppm in the finished product.

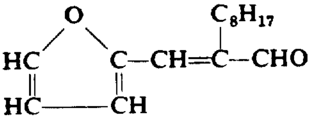
G.R.A.S. F.E.M.A. No.2809.

Prod.: by direct esterification of *n*-Octanol with Formic acid, e. g. in presence of Acetic anhydride.

26-642; 35-404; 61-72; 163-229; B-II-22;
NOTE: The *secondary*-Octyl formate is listed in this work under the title:
*alpha*-Methyl-*n*-hexyl carbinyl formate.
(2059).

## 2423: alpha-OCTYL FURFURACROLEIN

*alpha-n*-Octyl-*beta-2*-furylacrolein.



$C_{15}H_{22}O_2 = 234.34$

Viscous yellowish oil. Sp.Gr. 0.97.
B.P.~286° C.

Almost insoluble in water, soluble in alcohol, miscible with oils.

Very faint, sweet-oily, herbaceous-caramellic odor of considerable tenacity.

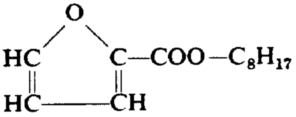
Although this chemical has been suggested as a fragrance material, it is the author's opinion that it has little or no mission in creative perfumery. It has no unusual notes or olfactory virtues to offer, but it may behave like a fixative with a mild, blending odor effect in woody or herbaceous fragrance types, or it may be an experimental modifier for the Amylcinnamic aldehyde in a Jasmin base.

Prod.: by condensation of Furfural and Decanal in mild alkaline solution.

31-40; 93-151;

## 2424: n-OCTYL FUROATE

*n*-Octylfuran-*alpha*-carboxylate.
*n*-Octyl pyromucate.



$C_{13}H_{20}O_3 = 224.30$

Colorless liquid.

Practically insoluble in water, soluble in alcohol, miscible with oils.

Mild, balsamic-sweet and remotely fruity odor of considerable tenacity.

This ester has been suggested for use in perfumes and flavors. The author has no report of its use in flavor compositions, but it is conceivable that it could be used in perfume compositions.

Its overall odor type and performance is quite similar to that of Octyl benzoate, which is primarily a fixative with possible use in Oriental, woody and heavy floral-balsamic fragrance types.

Prod.: by azeotropic esterification of *n*-Octanol with Furan-2-carboxylic acid.

## 2425: OCTYL HEPTIN CARBONATE

*n*-Octyl octynoate.

$CH_3(CH_2)_4C{\equiv}C{-}COO{-}C_8H_{17}$

$C_{16}H_{28}O_2 = 250.38$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol.

Oily-green, mildly leafy and somewhat fatty odor of considerable tenacity. Less Violet-leaf-like than the lower homologues of these esters.

This acetylenic ester has been suggested for use in perfume compositions but it probably had a very short life. By the time it became available, newer and much more interesting "green" odor chemicals had become commercially available, and it seems most likely that the title ester and many of its relatives will be materials of the past, curiosities on the shelf, if they ever reached the perfumer's shelf at all.

Prod.: e. g. by reacting Sodium heptyne with Octyl chloroformate.

163-59;

## 2426: OCTYL HEPTOATE

*n*-Octyl heptanoate.
Octyl heptylate.
Octyl oenanthate (old, misleading name).

$CH_3(CH_2)_7{-}OOC(CH_2)_5CH_3$

$C_{15}H_{30}O_2 = 242.41$

Colorless liquid. Sp.Gr. 0.87. B.P. 290° C.

Insoluble in water, soluble in alcohol and oils.

Oily-fruity, mildly green and fresh odor resembling the odor of unripe fruit. The oily notes are sweet and rather pleasant.

This ester has probably no mission in perfumery, but it does find some use in flavor compositions.

Traces are used in imitation Cherry, Malt, Mulberry, Nut, Coconut, Plum and various fruit complexes, Citrus blends, etc.

Concentrations are usually as low as 0.5 to 2 ppm in the finished product.

At that level, the taste is rather bland, and the effect hardly more than fixative. However, it serves as a good blender and has satisfactory effect where the flavored product may be exposed to heat during processing (baked goods, etc.). It may add to the "creamy" taste in Malt flavors as part of an Ice cream or Treacle flavor, or it may round-off a fruity complex.

Prod.: by azeotropic esterification of *n*-Octanol with Heptanoic acid.

G.R.A.S. F.E.M.A. No.2810.

7-305; 35-61; 35-404; 163-59; 163-229;

## 2427: OCTYLIDENE ACETONE

Undecen-*3*-one-*2*.
*3*-Undecen-*2*-one.
Methyl nonenyl ketone.

$CH_3(CH_2)_6CH{=}CH{-}CO{-}CH_3$

$C_{11}H_{20}O = 168.28$

Pale yellowish or almost colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet and oily-herbaceous, slightly fruity odor of moderate tenacity.

This ketone has been suggested for use in Jasmin compositions as a modifier for Amylcinnamic aldehyde, or in Gardenia and other heavy florals, where herbaceous-fruity notes are desirable and compatible with the fragrance picture.

The material is very rarely offered under its proper chemical name, but it has been incorporated in several successful specialties over the past few decades. To the creative perfumer, it is practically unknown, and it does not seem to grow in popularity, since no company has made an effort to promote it.

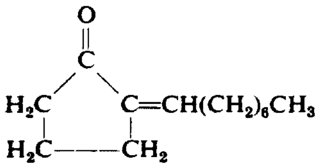
It is interesting to note that the title material can be hydrogenated to Methyl nonyl ketone (see that monograph) from which Methyl nonyl acetaldehyde used to be prepared.

Prod.: by condensation of Octaldehyde (Octanal) and Acetone.

7-305; 31-84; 163-59;

## 2428: alpha-OCTYLIDENE CYCLOPENTANONE

*2*-Octylidene cyclopentanone.



$C_{13}H_{22}O = 194.32$

Pale straw-colored or very pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils.

Floral and fruity, rather heavy and powerful, Jasmin-like, warm and discretely spicy odor of moderate tenacity.

This higher homologue (2 Carbon atoms higher) of *iso*-Jasmone has been suggested for use in perfume compositions. Its tenacity is slightly superior, but its odor type not quite as desirable as the conventional *iso*-Jasmones.

The material can be manufactured at a very attractive price, but it is rarely offered commercially under its proper chemical name.

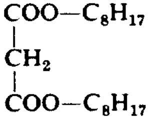
For novel Jasmin notes, for modifications of the pungent-floral theme in bases and finished fragrances, this ketone should have some future, if it were only made freely available.

Prod.: by condensation of Cyclopentanone with Octanal (Aldehyde C-8). (French patent No. 779789 of L. Givaudan Cie.).

31-86;

## 2429: n-OCTYL MALONATE

Di-*n*-octyl propane dioate.
Dioctyl malonate.



$$\begin{array}{l} COO{-}C_8H_{17} \\ | \\ CH_2 \\ | \\ COO{-}C_8H_{17} \end{array}$$

$C_{19}H_{36}O_4 = 328.50$

Colorless viscous liquid. Sp.Gr. 0.93.
B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

When absolutely pure, the ester is virtually odorless, but commercial samples have usually shown some degree of oily-fatty or bland-fruity odor.

The title ester has at one time been used as a diluent for Oakmoss resinoid and for other solvent purposes in perfumery, but the author believes that it is practically obsolete as a perfumery solvent, and that it has probably never been used as an odorant chemical.

It is briefly mentioned to complete the description of the many various types of solvents used – or formerly used – in perfumery.

Prod.: by direct esterification of *n*-Octanol with Malonic acid.

163-59;

## 2430: n-OCTYL OXYACETALDEHYDE

*beta*-Hydroxyacetaldehyde, Octylether.

$C_8H_{15}{-}O{-}CH_2{-}CHO$

$C_{10}H_{18}O_2 = 170.25$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful oily-green odor, sweet and green floral in dilution, the oily notes being fresh-nut-like, the green notes sweet, vegetable-like, with moderate tenacity.

This oxyaldehyde (ether) is one of the less popular of the series which was "revived" by the appearance of several oxyaldehydes and their acetals in 1967.

The acetals have apparently been more successful, and part of the reason could be the superior stability, another reason could be the more "subdued" odor character in the acetals, making them more attractive on the first encounter or experiment.

The title aldehyde would be used at the level of one percent or less up to a maximum of two percent in a fragrance, possibly higher in a base. It is rarely offered commercially, and the perfumers need more experimenting with this item before one can make any statements about the future prospects of the aldehyde.

Prod.: from Bromoacetal plus Potassium octylalcoholate, followed by acid hydrolysis of the resulting acetal.

See also: *2*-Hexoxyacetaldehyde dimethyl-acetal.

## 2431: OCTYL PELARGONATE

Octyl nonanoate.
Octyl nonylate.

$CH_3(CH_2)_7{-}OOC(CH_2)_7CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Peculiar earthy-floral, and oily citrusy odor of excellent tenacity.

The odor characteristics of this ester do not invite the perfumer to much experimenting. Although the overall odor of the chemical itself is rather weak, it can supply quite an amount of tonalities, not always desirable at the same time.

With proper blending, however, the ester can be directed in the wanted area, it may supply pleasant mushroomy-earthy notes with Vetiver and Oakmoss, while it may add oily-citrusy notes to a Bergamot composition, and warmth and green-earthy undertones in a Rose.

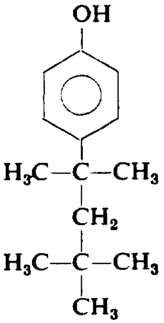
In brief, the title material is certainly dispensable, but it could be of some use if it were commonly available.

Prod.: by azeotropic esterification of *n*-Octanol with Nonanoic acid.

163-229; 163-367;

## 2432: OCTYL PHENOL

*para*-Octyl phenol.
The Octyl-radicle is almost exclusively in the *para*-position, but it consists of mostly branched-chain Octyl isomers, one of which is shown below:
*4-(para*-Hydroxyphenyl)-*2:2:4:4*-tetramethylbutane:



$C_{14}H_{22}O = 206.33$

White powder, melting at 86° C. B.P. 282° C. The *n*-Octyl isomer has B.P. 292° C.

The title material is almost insoluble in water, soluble in alcohol and most oils, but very poorly soluble in aqueous alkali, contrary to lower alkyl phenols which are soluble in aqueous alkali.

The title material is not a perfume chemical as such, but it serves as an intermediate in the manufacture of Octyl cyclohexanone and other useful odorous chemicals. The title material is therefore available to perfumers in such manufacturing companies, and it may occasionally be used for special perfumery projects.

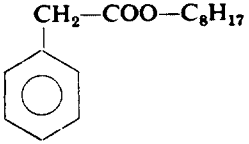
The phenol has a faint, dry-medicinal odor, but not as choking or distinctly "phenolic" as that of Phenol or Cresol. It has therefore found use in certain types of detergent fragrance, where a mild, but unquestionable "medicated" note is desirable to emphasize a disinfectant effect, or similar special effect, attached to that detergent product.

The lower alkyl phenols, e. g. Amyl and Butyl – also raw materials for the manufacture of perfumery ketones, etc., are more frequently used for the above purpose.

68-423;
see also: Journal of American Chemical Society 1948, vol. 70, page 1474.

## 2433: n-OCTYL PHENYLACETATE

*n*-Octyl-*alpha*-toluate.



$C_{16}H_{24}O_2 = 248.37$

Colorless viscous liquid. B.P. 315° C.
Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Mild, but very tenacious, sweet-floral odor of woody-Orange-Rose type. The Orange character seems to come from oily-sweet notes which may be concealed under Rose-honey notes if the ester is poorly balanced (i. e. contains one or both of the parent chemicals in the manufacture of the ester).

The ester is rarely used in perfumes, but it does find some application in flavors, e. g. imitation Apple, Banana, various berry complexes, Grape, Peach, Pear, etc.

The concentration of this ester in the finished product is normally very low, about 1 to 5 ppm.

The flavor at that level is barely perceptible as sweet, mildly fruity, but again, if the ester is not pure, the flavor is severely influenced by traces of Phenylacetic acid or Octyl alcohol, both of which are more penetrating at that level.

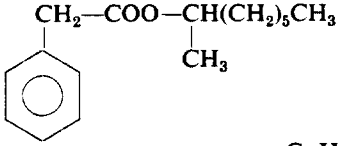
Prod.: by azeotropic esterification of *n*-Octanol with Phenylacetic acid.

G.R.A.S. F.E.M.A. No.2812.

## 2434: n-secondary-OCTYL PHENYLACETATE

Methyl hexyl carbinyl-*alpha*-toluate.
*2*-Octanyl phenylacetate.

NOTE: The literature occasionally claims that the title material is Ethyl amyl carbinyl phenylacetate, but the author believes that the Methyl hexyl carbinyl phenylacetate is more common.



$C_{16}H_{24}O_2 = 248.37$

Colorless viscous liquid. B.P. 312° C.
Sp.Gr. 1.02.

Insoluble in water, soluble in alcohol and oils.

Oily-herbaceous, slightly earthy-woody and sweet-spicy odor of considerable tenacity.

This ester does not seem to have enjoyed much popularity in perfumery or flavor creation. There has been much confusion as to its exact chemical identity, since "Octyl alcohol" industrially often means *2*-Ethylhexanol, while the perfume chemists generally expect the *n*-Octanol. Further complications occur when "*secondary-*" Octyl alcohol enters the picture. The result is a general confusion and it is followed by an almost complete loss of interest in the material, particularly when samples arrive with identical labelling and distinctly different odor type.

The perfumers will not suffer any great loss in living without this item.

Prod.: by azeotropic esterification of Methyl hexyl carbinol with Phenylacetic acid.

35-404;

## 2435: OCTYL PROPIONATE

$CH_3(CH_2)_7—OOC—CH_2—CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid. Sp.Gr. 0.87. B.P. 226° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet, oily-waxy and fruity-herbaceous odor, overall a relatively pleasant complex with many notes resembling food or condiment products. The tenacity is moderate.

This ester has been suggested as a supporting note in warm-herbaceous and floral herbaceous fragrance types, and it blends very well in Lavender, Lavandin, Rosemary, Juniperberry, Myrtle, Laurel and Bayleaf oils. Although its odor has very little in common with Myrtle, it lends a pleasant support of softness, and reduces the cineolic notes in Myrtle oil.

For general use as a modifier in novel types of Fougère, the title ester offers interesting possibilities.

It finds some use in flavor compositions, e. g. in Honey, Pineapple, various berry compositions, citrus complexes, Melon, Champignon, etc, but normally at very low concentrations – equal to 0.5 to 5 ppm in the functional product.

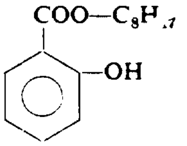
Prod.: by azeotropic esterification of *n*-Octanol with Propionic acid.

G.R.A.S. F.E.M.A. No.2813.

33-620; 35-404; 163-59; 163-229;

## 2436: OCTYL SALICYLATE

*n*-Octyl-*ortho*-hydroxybenzoate.



$C_{15}H_{22}O_3 = 250.34$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Practically odorless when pure.

This ester has been offered as a perfume material, but since it does not contribute any interesting notes, and since it is more expensive than the conventional solvents and odorless "blenders", there is very little demand for the material.

Its fixative effect is not distinctly superior to that of many common materials, but the title ester does lend a mild, floral note to a composition if used at relatively high percentage, e. g. 10-20% in mild floral types, Lilac, Muguet, etc. It is not as sweet, floral or odorous as Benzyl salicylate.

Briefly, the material is definitely dispensable.

Prod.: by azeotropic esterification of *n*-Octanol with Salicylic acid.

163-59;

## 2437: OCTYL-n-VALERATE

*n*-Octyl-*n*-pentanoate.

$CH_3(CH_2)_7—OOC(CH_2)_3CH_3$

$C_{13}H_{26}O_2 = 214.35$

Colorless liquid. B.P. 250° C. Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Fruity and relatively diffusive, Apple-Banana-like odor with fresh-"aldehydic" notes and moderate tenacity.

This ester is rarely, if ever, used in fragrances.

It finds a little use in flavor compositions as a fixative in Apple and Banana imitations, and in various fruit complexes.

The title material is not specifically mentioned in the American G.R.A.S. list, but since the *iso*-valerate is listed, there is some justification in assuming that it covers the *n*-ester.

*n*-Valerates and *iso*-Valerates are often mentioned indiscriminately in (perfumery) literature, and it has become more or less common practice to use the term "Valerate" for the *iso*-Valerate.

Prod.: by azeotropic esterification of *n*-Octanol with *n*-Valeric acid.

7-305; 8-404; 33-933; 163-59;
see also: Octyl-*iso*-valerate, next monograph.

## 2438: n-OCTYL-iso-VALERATE

*n*-Octyl-*3*-methylbutyrate.

$CH_3(CH_2)_7{-}OOC{-}CH_2{-}CH(CH_3)_2$

$C_{13}H_{26}O_2 = 214.35$

Colorless liquid. Sp.Gr. 0.86. B.P. 245° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, fatty-fruity, herbaceous odor of moderate tenacity. The herbaceous notes are rather heavy, almost spicy, and the terminal notes are "powdery" resembling the dryout of root-like odors.

This ester is somewhat more common than the *n*-Valerate, and it is used to some extent in fragrance compositions. In "sophisticated" Pine bases, in woody and herbaceous fragrances, with Oakmoss and Vetiver, it gives rather useful effects and novel notes.

The ester is more commonly used in flavor compositions, mainly for imitation Apple, Banana, Butter, Cherry, Grape, Honey, Nut, etc. and in fruit complexes ("tutti-frutti"), berry compositions, citrus notes, etc.

The concentration is normally about 0.5 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2814.

Prod.: by azeotropic esterification of *n*-Octanol with *iso*-Valeric acid.

33-932; 33-934; 35-404; 163-59; 163-229;

## 2439: OCTYNE

*1*-Octin.
*1*-Octyne.
*n*-Hexyl acetylene.
Caprylidene.
*alpha*-Hexyl acetylene.

$CH{\equiv}C(CH_2)_5CH_3$

$C_8H_{14} = 110.20$

Colorless mobile liquid. Sp.Gr. 0.74.
B.P. 137° C.

Insoluble in water, soluble in alcohol and oils.

Although the title material is not truly a fragrance material, it has occasionally served as component in perfumes for special purposes, e. g. industrial masking odors, etc.

Octyne is an intermediate chemical in the manufacture of a number of more useful perfume chemicals, and it is thus available to perfumers in the manufacturing companies.

Its volatility puts it into a class of "lifting" materials, but its odor type is not exactly desirable. Yet, it is not as "gassy" as the Styrene family, and not as "gasoline"-like as the Olefins or Paraffins. It is ethereal and sweet, of very poor tenacity, warm and remotely resembling the odor of Myrcene in its warm spiciness.

Prod.:

1) from Methyl hexyl ketone and Phosphorous pentachloride followed by hydrolysis and treatment with Sodamide.
2) by Bromination of *n*-Octene (commercially available) followed by debromination of the Dibromo octane with dry Potassium hydroxide in mineral oil.

5-243; 156-10; 66-264;
See also: *1*-Octene 2421.

## 2440: OLEIC ACID

Elain. (The commercial grade contains about 10 to 12% saturated acids).
Oleinic acid.
*9*-Octadecenoic acid.
*trans*-Elaidic acid.

$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$

$C_{18}H_{34}O_2 = 282.47$

Almost colorless or very pale yellowish oily liquid, solidifying in the cold to an opaque, crystalline mass. M.P. 13° C. Sp.Gr. 0.90. B.P. approximately 340° C. The acid decomposes if heated beyond 80° C. at atmospheric pressure, becoming dark, acquiring a rancid odor by oxidation.

A truly pure acid has very little odor, very little color and very little taste, but most commercial grades, even the "high-grade" materials have a faint, bland-oily odor, sweet-oily taste and usually a faint color. Only "high-grade" material, normally sold under various trade names, is suitable for perfumery purposes.

The title material finds limited use in perfume compositions as part of the "flower-wax"-like odor in artificial flower absolutes, floral bases, etc. particularly in Tuberose, Gardenia, etc.

Oleic acid is also used in flavor compositions for imitation Banana (mouthfeel, more than flavor), Butter, Cheese, Honey and in various spice blends. The concentration is normally about 1 to 30 ppm, in some cases much lower, in Banana often higher. Since the acid is also used partly as a fixative, higher concentrations are found in flavors used for baked goods and Icecream.

G.R.A.S. F.E.M.A. No.2815.

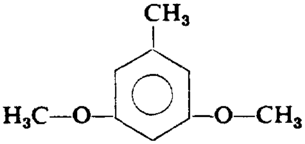
Prod.:

1) by isolation from natural products by fractionated low-temperature crystallization of natural acids or Methylesters of same.
2) by hydrolysis of animal and vegetable fats and oils.

66-639; 100-753; B-II-463; 26-644;

## 2441: ORCINOL DIMETHYLETHER

*3,5*-Dimethoxytoluene.
*1*-Methyl-*3,5*-dimethoxybenzene.
*5*-Methylresorcinol dimethylether.



$C_9H_{12}O_2 = 152.20$

Colorless liquid. B.P. approximately 245° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm and sweet, nut-like, earthy-mossy odor of moderate tenacity.

This rare material has been suggested for use in perfume compositions as supporting note for Oakmoss and Vetiver, and as a novel note in Chypre, Fougère and Oriental fragrance types.

Its type is primarily Oakmoss, and it performs excellently with all types of Oakmoss extract, adding sweetness and warmth without adding any perceptible "chemical" notes. The material is also interesting in combinations with Nonanolide and with the Hexenols. New and attractive effects are obtained in Hyacinth and Hay odors as well as "Nut" types with Oakmoss and Vetiver, Hydroquinone dimethylether, Octanolide etc.

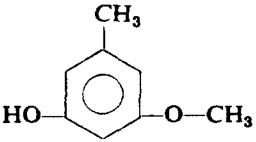
The ether is used in some countries in flavor compositions for imitation Hazelnut and Walnut, but it is not listed in the U.S.A. as G.R.A.S.

Prod.: from Orcinol in weak aqueous alkali with Dimethylsulfate at controlled temperature.

68-474; private experiments;

## 2442: ORCINOL MONOMETHYLETHER

*3*-Methoxy-*5*-hydroxytoluene.
"Monomethylorcin".
*5*-Methoxy-*ortho*-cresol.
*3*-Hydroxy-*5*-methoxytoluene.



$C_8H_{10}O_2 = 138.17$

White crystals or colorless needle-like crystals. M.P. 62° C. B.P. 259° C. Sp.Gr. 1.11 (supercooled).

Very slightly soluble in water, soluble in alcohol and oils.

Dry-woody-tarry, also Walnut-like odor of good tenacity. Although not nearly as dry as the cresols, this material is less sweet than the -dimethylether (see previous monograph) and less Nut-like. However, it is still an Oakmoss-type material, and it finds use as such in perfume compositions.

This phenolether is very rarely offered as such but may be a very common ingredient in "specialties" used almost every day by the working perfumer. There are few good Oakmoss chemicals, but this should be included as one of them. It is most unfortunate that the material is not made available to the perfumers – except the few perfumers working with a manufacturer of this chemical – because it could be utilized far beyond its suggested applications, very incompletely mentioned in literature.

The fact that the material is a phenol should not scare the perfumer from experimenting, because the power of the title material may in many cases compensate for its possible drawbacks at higher concentrations. It is furthermore interesting to note that this Monomethylether is much more powerful than the -dimethylether (see previous monograph), while the latter has the advantage of causing no discoloration in alkali – only some discoloration when exposed to air or direct daylight.

The title material exists – under acid conditions – in the volatile part of Oakmoss extract, and is probably part responsible for the fact that the "decolorized" Oakmoss extract often causes more discoloration in a perfume (or cosmetic product) than the natural, green extract – in which the title ether is not nearly as concentrated.

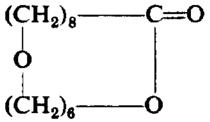
Prod.: by regulated Methylation of Orcinol with Dimethylsulfate in weak aqueous alkaline solution.

The material is generated in Nature by decarboxylation of Evernic acid, a major component of Oakmoss (extract).

7-303; 68-474; 90-384;

## **2443: 10-OXAHEXADECANOLIDE**

"Oxalide" (Takasago Perfumery Co. Ltd.).
"Musc 906" (Takasago).
A Chromane type, macrocyclic musk.



$C_{15}H_{28}O_3 = 256.39$

Colorless, viscous liquid. Sp.Gr. 0.99.

Practically insoluble in water, soluble in alcohol and miscible with all perfume materials.

Sweet, soft and extremely tenacious, discretely animal-musky odor. Although the title material has notes resembling Versalide and Ethylene brassylate, it is overall more luxurious in its uniformity and absolutely free from fatty or acid notes.

It is generally difficult to estimate the power of musks, but the tenacity of the title material is approximately three times better than that of Ethylene brassylate, and its power – in actual use – unsurpassed by any other musk in that price level.

Among relatively few synthetic musks, this material has unquestionable "wearability" on the human skin. Its effect can only be justly evaluated by studying the effect of a perfume containing the musk, in use on human skin. The power and radiance will show up quite perceptibly, and the difference between an "ordinary" musk and a truly outstanding musk will become evident.

This musk was developed only a few years ago after an intense search of a macrocyclic musk with Cyclopentadecanolide-like effect and at low cost. The title material is priced slightly above Ethylene brassylate, and this should eliminate the last possible objection against the new musk.

With an odor between that of Cyclopentadecanolide and Ambrettolide, and an unquestionable exalting effect, this material offers one of the most tempting tools in the hands of the curious, creative and imaginative perfumer – and he can hardly fail in his experiments with it.

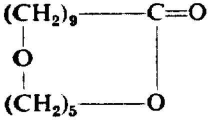
Two isomers of subject musk are commercially available from another manufacturer, and they are described in the following monographs, one of these musks is also manufactured by other companies. Although generally well known, the Oxahexadecanolide musks are generally offered under trade name.

Prod.: many methods, see also: 156-261 and 156-264;

Takasago Perfumery Company, Ltd. Tokyo, Japan. Material and data, Jan. 1968.

## 2444: 11-OXAHEXADECANOLIDE

"Musk R-1" (Naarden, N.V., Holland).
A Chromane type, macrocyclic musk.



$C_{15}H_{28}O_3 = 256.39$

Opaque crystalline mass. M.P. 35° C.

Almost insoluble in water, soluble in alcohol and oils. The solubility in diluted alcohol is superior to that of Cyclopentadecanolide.

The material may remain supercooled as a viscous, colorless liquid if it has been melted and not exposed to cold shock.

This musk was developed in the 1930's, but it took several decades to complete the synthesis and bring it to such perfection that the material could be manufactured at an attractive cost – in competition with the famous Cyclopentadecanolide, which until then had enjoyed almost monopoly in its field.

The title material is an outstanding fixative and an exquisite musk odor with a pleasant note resembling Ambrette-seed oil. The effect of this musk is only fully understood after evaluation of a perfume solution in which the musk has been used, or an evaluation of a "pre-fixed" perfume alcohol with 0.01% of the title material.

Perfumers have generally agreed that this musk is one of the closest approaches to the Cyclopentadecanolide so far available.

This musk is used in perfume compositions at concentrations of 0,5% or higher, although lower concentrations are known to have had perceptible effect. After proper ageing, the alcoholic perfume solution will show the effect of the musk at its best when applied to the human skin. This is where the difference appears between the "ordinary" musks and the truly unique musks.

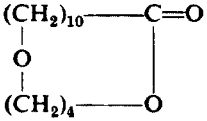
The use of this material in minute traces in beverages, chewing gum and other flavored products is known, but the correct dosage in flavors is much more important than in perfumes, in fact, the effective level and the "pleasant-level" constitute extremely narrow limits for its application in flavors. The suggested use level is normally well below 0.1 ppm in the finished product, and lowest in beverages. The desirable effect is that of a simultaneous mellowing and enhancing of the flavor, – a true, but almost unidentifiable "bouquetting".

Prod.: many methods – see also: 156-261; 156-251;

Naarden (Holland) data sheet and material, 1966.
Parfumerie, Cosmetique, Savons, Nov. 1965, pages 475-480.

## **2445:** 12-**OXAHEXADECANOLIDE**

"Cervolide" (N.V. Chem. Fabr., Naarden, Holland).
"Hibiscolide" (Roure-Bertrand)
*16*-Hydroxy-*12*-oxahexadecanoic acid, *omega*-lactone.
A Chromane-type, macrocyclic musk.



$C_{15}H_{28}O_3 = 256.39$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, tenacious and intensely musky odor. Generally considered less powerful and less tenacious than Cyclopentadecanolide, and it does not have the attractive and highly appreciated "Ambrette-seed"-like note as found in the more expensive isomer from the same manufacturer (see *11*-Oxahexadecanolide, earlier monograph).

However, in competition with the equally priced Ethylene brassylate, the title material is undoubtedly superior, "cleaner", and absolutely free from fatty or "oily" notes.

It seems that the composing of selected fractions from the final vacuumdistillation of these musks is the most important part of their manufacture. Many companies can make macrocyclic musks and many companies can make Methylionones, but if the material is not composed under control of a trained nose, of a person who himself understands and appreciates the perfumery effect of the material, then the resulting chemical may come out in a quality liked by few, disliked by many.

This musk should appeal to a perfumer as the type of musk one could use in almost any type of perfume, including soap perfumes and other so-called "low-cost" fragrances. Concentrations below 1% may have perceptible and satisfactory effect, while much higher concentrations may be used where outstanding retentiveness (modern soap perfumes) is a desirable feature. It blends particularly well with the Methylionones, Undecanolide, Nonanolide, Cinnamic alcohol etc. for such purposes.

Today's perfumer is unfortunately liable to look strongly at the immediate price of a musk, but only experiments can show him what it actually costs to introduce a desirable musk effect. And the effect obtainable with macrocyclic musks of the subject type can not be imitated with any (larger or smaller) amount of a Nitromusk.

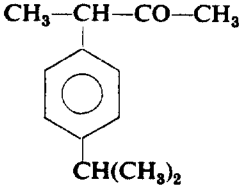
Unless perfume chemistry research comes up with methods of reducing the cost of this type musk, the title material and its isomer cousins should have a very successful and long future of increasing use in perfumery.

Prod.: many methods, see also 156-261 and 156-264;

See: N.V. Naarden – data sheet 1966 ("one of Naarden's seven").

## **2446:** 1-**OXO**-2-**METHYL**-2-(para-iso-**PROPYLPHENYL**)-**ETHANE**

*para-iso*-Propylphenyl ethyl methyl ketone.
*para*-Cymyl ethyl methyl ketone.
*2*-(*para-iso*-Propylphenyl)-*3*-butanone.



$C_{13}H_{18}O = 190.29$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and woody-floral, delicately green odor of good tenacity. The overall odor bears some resemblance to that of Cyclamen aldehyde.

This ketone has been suggested for use in perfume compositions, and it has been incorporated in several successful specialties. The material is rarely available under its proper chemical name, and it also appears to have lost much of its popularity, perhaps because of the fact that the material has not always been commercially available.

In floral and floral-woody fragrance types, it blends well with the Ionones and Methylionones, with Styrax and Cinnamic alcohol, with the "rose" alcohols, etc.

Prod.: (several methods) e. g. by hydrogenation of *1*-Methyl-*1*-phenylpropan-*2*-ol. The secondary alcohol can be obtained by Grignard type synthesis.

## 2447: PALMITIC ACID

Hexadecanoic acid.
*n*-Hexadecylic acid.
Cetylic acid.

$CH_3(CH_2)_{14}COOH$

$C_{16}H_{32}O_2 = 256.43$

Colorless or white flaky crystals. M.P. 64° C. B.P. over 300° C. (decompos.). Sp.Gr. 0.85 (liquid).

Insoluble in water, approximately 10% soluble in alcohol, somewhat better in hot alcohol. Soluble in most perfume and flavor materials.

Virtually odorless when absolutely pure. The material is rarely, if ever, used in perfume compositions for olfactory purposes.

The taste is very bland, and the effect is really more a mouthfeel than an aroma or flavor.

This acid finds some use in flavor compositions for imitation Butter and Cheese at amazingly low concentrations. The author feels that the effect could hardly be any aromatic effect, but barely that of a "mouthfeel" or texture effect in the above flavor types and the corresponding functional products.

Concentrations are given at approximately 1 ppm in the finished consumer products.

G.R.A.S. F.E.M.A. No.2832.

Prod.: from Palm kernel oil, Olive oil, Japan wax or Chinese vegetable tallow by saponification of the natural glycerylesters.

26-464; 66-578; 100-768; 160-1138; B-II-370;

## 2448: PARMAVERT

*2*-Nonyn-*1*-al dimethylacetal.
Hexyl propiolic aldehyde dimethylacetal.
This material is listed under its trade name because it was known for some time under that name and not under the inconvenient chemical name, only recently revealed.

$CH_3(CH_2)_5C{\equiv}C{-}CH(OCH_3)_2$

$C_{11}H_{20}O_2 = 184.28$

Colorless oily liquid. B.P. 225° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, floral-green, sweet and Violet-leaf-like odor of moderate to poor tenacity.

This acetal was marketed several years ago under the name Parmavert and it was very well received. In spite of the fact that it may never become a "volume item" on account of its power, it will undoubtedly find its place in a great variety of fragrance types, other than Violet and leaf-types.

Its main asset is its natural sweet-weedy odor, which falls equally well into a Violet and Narcisse as in a Citrus, Fougère or Moss-type fragrance. It performs excellently with Mimosa, Cyclamen aldehyde, Geranium oil, Oakmoss, Galbanum, Styrallyl propionate, Gardenia bases, etc., briefly, it has something to offer which is not found in any other single chemical.

Prod.: from *1*-Octyne by reaction with Ethyl-*ortho*-formate directly to the acetal. Octyne is obtained from Octene via bromination and debromination.

66-504; 156-7; 156-8; 163-366;
(sample: Compagnie Parento, Inc. U.S.A.).

## 2449: PENTADECANAL

"Aldehyde C-15, true".
Pentadecanal-*1*.
Pentadecyl aldehyde.

$CH_3(CH_2)_{13}CHO$

$C_{15}H_{30}O = 226.41$

White waxy-crystalline mass melting at 25° C. B.P. 279° C.

Insoluble in water, soluble in alcohol and oils.

Polymerizes upon exposure to air and daylight, becomes solid and odorless.

Very faint, but delicately fresh-floral odor of good tenacity.

This aldehyde, only rarely offered from the regular manufacturers of perfume chemicals, is occasionally used in perfume compositions as part of a floral base or part of a floral topnote, aldehydic-green or aldehydic-fruity topnote.

It blends excellently with Methylnonylacetaldehyde and has a mellowing effect upon that material, but in general, the title aldehyde is dispensable in modern perfumery.

Prod.: by oxidation of Pentadecanol (see next monograph).

66-477;

## 2450: PENTADECANOL

Pentadecanol-*1*.
*n*-Pentadecyl alcohol.
Alcohol C-15, true.

$CH_3(CH_2)_{13}CH_2OH$

$C_{15}H_{32}O = 228.42$

White or colorless crystalline leaves, or waxy mass. M.P. 45° C.

Insoluble in water, soluble in hot alcohol and oils, poorly soluble in cold alcohol.

Very faint, bland-waxy and discretely floral odor of excellent tenacity. An absolutely pure material is reported to be virtually odorless.

The title alcohol has occasionally been used in perfume compositions as part of floral bases, artificial flower absolutes, etc.

There are, however, many, and also some better, materials for such purposes, and the title material is not truly needed in a creative perfume laboratory, although there are opinions that no material should be banned from availability to the creative perfumer. Which is, in its true effect, an ideal situation. But extremely rare, and not favored by the financially minded departments of a company.

Prod.: via Myristic acid and the Cyanide (Pentadecanoic nitrile) to the Pentadecanoic acid via Ethylester and reduction to the title alcohol.

26-648; 160-1140; 163-230; B-I-429;

## 2451: PENTADECYL ACETATE

Acetate C-15, true.

$CH_3(CH_2)_{13}CH_2—OOC—CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless liquid, solidifying in the cold to a waxy mass. M.P. 11° C. B.P. near 300° C.

Insoluble in water, soluble in alcohol and oils.

Faint, but sweet and delicate, ethereal-winey, oily odor. Good tenacity.

This ester has occasionally been used in perfume compositions as supporting note in sweet-Ambre or Ambrette-seed like bases, along with Cognac oil, Dodecyl propionate, Decenyl propionate, etc.

It has also been used in floral bases, such as Rose, Narcisse, Lily, Muguet, etc. as a mellowing ingredient.

Its perfumery value is very limited, and most laboratories are forever living completely without it, and not missing a great material.

Prod.: by azeotropic type esterification of Pentadecanol with Acetic acid.

26-648; 31-122; B-II-136;

## 2452: 4-PENTENOIC ACID

Allyl acetic acid.

$CH_2{=}CH{-}CH_2{-}CH_2{-}COOH$

$C_5H_8O_2 = 100.12$

Colorless liquid. Sp.Gr. 0.98. B.P. 189° C.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

This acid is only rarely used in perfume compositions, mainly in fruity bases and certain artificial essential oils.

It finds use in flavors on account of its sour-caramellic taste, pleasant at levels below 10 ppm, and including an almost sweet after-taste. Higher concentrations have acrid taste and repulsively acid odor, pungent and irritating.

Traces, equivalent to 1 to 5 ppm, are used in imitation Butter flavor and in various fruit flavor complexes, e. g. Apple, Pineapple Apricot and Strawberry.

G.R.A.S. F.E.M.A. No.2843.

Prod.: from Allyl bromide via Malonic ester synthesis or via Acetoacetic ester synthesis.

26-394; 66-637; 160-1148; B-II-425;

Note: Other Pentenoic acids are listed in this work under:

Angelic acid, (238),

Tiglic acid. (2929).

## 2453: PENTENOIC ACID, NITRILE

Allyl acetonitrile.
*4*-Pentene nitrile.
*3*-Butenyl cyanide.
Allyl carbinyl cyanide.

$CH_2{=}CH{-}CH_2{-}CH_2{-}CN$

$C_5H_7N = 81.12$

Colorless liquid. Sp.Gr. 1.18. B.P. 140° C.

Insoluble in water, soluble in alcohol and oils.

Powerful and pungent Mustard-like odor of poor tenacity. In concentrations higher than 1% (in odorless solvent) the vapors are strongly irritating, but at lower concentrations the odor can be evaluated without such effect.

Pungent and burning taste, Mustard-like effect in concentrations below 5 ppm. Unpleasant at higher levels.

This material has been used in artificial Mustard flavor but it is not specifically listed in the American G.R.A.S. list as permitted for food flavors.

It is not unusual for a creative and imaginative perfumer to use minute traces of such materials in certain fragrances in order to obtain a "lifting" effect, perhaps due to a "sharpening" of the olfactory receptacles by the slight irritation from pungent vapors. However, the "trick" does not always work to satisfaction, and it demands great skill and a delicate hand to dispense such unconventional "fragrance" materials.

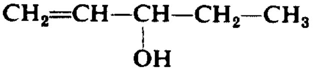
Prod.: from *3*-Butenyl bromide plus Cuprous cyanide.

26-394; 160-1148; B-II-426;

## 2454: beta-PENTENOL

*1*-Penten-*3*-ol.
Vinyl ethyl carbinol.
Ethyl vinyl carbinol.

Note: Three other Pentenols are known and commercially available, but the author believes that the title material is the material referred to in older perfumery literature:



$CH_2{=}CH{-}\underset{\displaystyle OH}{\underset{|}{CH}}{-}CH_2{-}CH_3$

$C_5H_{10}O = 86.14$

Colorless mobile liquid. Sp.Gr. 0.84. B.P. 115° C.

Powerful, gassy-green and very diffusive odor.

This alcohol has been used in perfume compositions as part of leafy-green topnotes, as a "lifting" ingredient, and in combination with Galbanum, Geranium and similar materials for powerful effects.

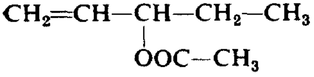
The alcohol has lost most of its importance since the Hexenols have become commercially available including many interesting esters, etc.

Prod.: from Acrolein and Ethyl magnesium iodide (by Grignard type reaction).

26-550; 163-369; B-I-443;

## 2455: beta-PENTENYL ACETATE

Ethyl vinyl carbinyl acetate.
*1*-Penten-*3*-yl acetate.
Vinyl ethyl carbinyl acetate.
See note under previous monograph.



$CH_2{=}CH{-}CH(OOC{-}CH_3){-}CH_2{-}CH_3$

$C_7H_{12}O_2 = 128.17$

Colorless liquid. B.P. 129° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and diffusive, green-fruity, somewhat pungent odor of poor tenacity. The fruitiness resembles that of Amyl acetate, but it is not nearly as sweet, the greenness is slightly gassy-leafy, Violet-like.

This ester has been used in perfume compositions as part of topnote bases, fruity-green bases, etc., often in combination with Geranium, Lavender, Citrus oils, etc.

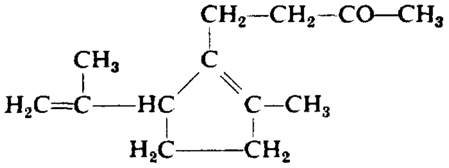
However, the ready availability of many excellent Hexenyl esters of far greater versatility in creative perfumery has largely made this ester dispensable, and it is reasonable to say that the title material is practically obsolete in perfumery.

Prod.: by azeotropic type esterification of *1*-Penten-*3*-ol with Acetic acid.

2-717;

## 2456: PENTIONE

*4*-(*2*-Methyl-*5*-*iso*-propenyl-*1*-cyclopenten-*1*-yl)-*2*-butanone.



$C_{13}H_{20}O = 192.30$

Pale yellowish, oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Woody and faintly citrusy odor with some resemblance to the odor of the Ionones, but inferior tenacity.

This ketone is included in the present work as one example of a series of chemicals commonly known as the Pentiones, made commercially available almost a decade ago, but never gaining much popularity among perfumers.

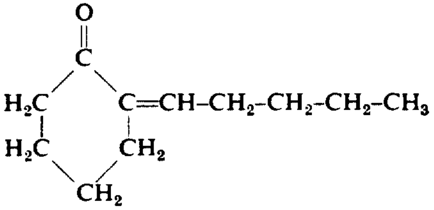
The title material is an empirical isomer of Ionone, and its structure bears some resemblance to those ketones. But the Pentiones were never met with much enthousiasm by the perfumers, and it is reasonable to state that they are almost obsolete in today's perfumery.

Various isomers and related derivatives were manufactured and they presented quite different odortypes, ranging from woody via floral to the warm-herbaceous, Labdanum-like or almost Citrus-like types.

(Hoffmann-laRoche, Inc.).

100-783; 163-369;

## 2457: 2-n-PENTYLIDENE CYCLOHEXANONE-1



$C_{11}H_{18}O = 166.27$

Colorless or pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils.

Warm and slightly spicy, Jasmin-like odor of excellent tenacity. Not as sweet as *iso*-Jasmone, but also less Celery-like in its warm-spicy character. Overall less floral than the most popular *iso*-Jasmones and Didydro jasmones, etc.

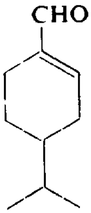
This ketone has been suggested for use in perfume compositions as a type of "Jasmone" for floral bases, topnote compositions, etc. It is rarely available under its proper chemical name, but it is used by various private manufacturers and included in certain specialties.

Prod.: by condensation of *n*-Valeraldehyde and Cyclohexanone.

163-250; see also D.R. patent No. 676171.

## 2458: PHELLANDRAL

*4-iso*-Propyl-*1*-cyclohexen-*1*-al.
*para*-Menthen-7-al.
Tetrahydro cuminaldehyde.



$C_{10}H_{16}O = 152.24$

Colorless mobile liquid. Sp.Gr. 0.94.
B.P. 174° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, but not pungent, green-herbaceous odor of spicy-condiment-like type. The odor is often classified as "resembling that of Cuminaldehyde", but the author finds that the odor of the title material is much milder and not at all repulsive even at high concentration. It has actually a sweeter character.

This material has been suggested for use in perfume compositions as a fresh-herbaceous, green note in Lavender, Chypre, Fougère and novel variations of the Oakmoss-fruity-green topnote complex, etc.

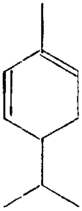
Prod.:

1) by isolation from Waterfennel oil (mainly *d*-Phellandral).
2) from *iso*-Propyl phenol via *iso*-Propyl-cyclohexanol to the ketone and via the Cyano-derivative to the acid, which is reduced to the title aldehyde, mainly the *dl*-isomer.

89-111; 95-133; 163-231; 163-370; 67-522;

## 2459: alpha-PHELLANDRENE

*2*-Methyl-*5*-*iso*-propyl-*1,3*-cyclohexadiene.
*para*-Mentha-*1,5*-diene.
*4*-*iso*-Propyl-*1*-methyl-*1,5*-cyclohexadiene.
*1*-*iso*-Propyl-*4*-methyl-*2,4*-cyclohexadiene.



*d*- and *l*-forms are known.

$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.85.
B.P. 175° C.

Insoluble in water, poorly soluble in diluted alcohol, soluble in alcohol, miscible in oils.

The material is relatively unstable under normal storage conditions, and particularly under acid conditions.

It tends to polymerize and decompose unless kept at low storage temperature, in a dark place and preferably under Nitrogen or $CO_2$-blanket.

When absolutely pure, the material has a pleasant, fresh-citrusy and peppery-woody odor with a discretely minty note. Poor tenacity. Commercial grades are often contaminated with Cymene or other Terpenes and display variable amounts of "kerosene-like" notes. The odor of the title material is overall less lemony than that of the *beta*-isomer.

This terpene is used in perfume compositions and in artificial essential oils of the Citrus type, Pepper, Geranium and certain other oils. Commercial grades may be used as part of odors for industrial masking purposes.

The title material finds some use in flavor compositions, mainly in Citrus and spice complexes to give "lift" to essential oils of those types, etc.

The normal use concentration is about 10 to 130 ppm in the finished consumer product.

The *alpha*-Phellandrene is generally preferred as a "peppery" odor while the *beta*-Phellandrene is more "citrusy". However, there has been some difficulties in obtaining both terpenes in regular supply.

G.R.A.S. F.E.M.A. No.2856.

NOTE: *beta*-Phellandrene is *not* included in that list).

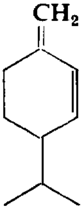
Prod.: The *laevo*-form is obtained by isolation from Eucalyptus numerosa and other Eucalyptus oils.

The title terpene is also obtained in the manufacture of synthetic Menthol.

26-648; 31-7; 87-94; 85-96; 100-790; 104-66; 104-222; 104-233; 106-283; 160-1150; 163-61; 163-231; B-V-129;

## 2460: beta-PHELLANDRENE

*1*-Methylene-*4*-*iso*-propyl-*2*-cyclohexene.
*1*(*7*),*2*-*para*-Menthadiene.
*3*-*iso*-Propyl-*6*-methylene-*2*-cyclohexene.
*d*- and *l*-forms are known.



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.85
B.P. 171° C. (*dextro*-) 178° C. (*laevo*-).

Insoluble in water, poorly soluble in alcohol, miscible with oils.

Peppery-minty, refreshing and slightly citrusy odor of poor tenacity.

In concentrations below 20 ppm the material has a pleasant peppery-warm taste, but at higher concentrations it is accompanied by a slightly burning mouthfeel. The taste is more minty, less citrusy, also more peppery than that of the *alpha*-isomer (see previous monograph).

The title terpene is rather unstable under normal storage conditions, and should be kept in a dark place preferably under Nitrogen or Carbon dioxide blanket to prevent deterioration and polymerization.

*beta*-Phellandrene is used to some extent in perfume compositions; the pure grade is preferred for artificial essential oils, Angelica, Pepper, Geranium, etc. The *alpha*-isomer is generally preferred for Bergamot and Lemon oil imitations.

Commercial grades are not suitable for such delicate work, and find use in industrial masking odors and low-cost detergent perfumes, Citrus bouquet for household product fragrances, etc.

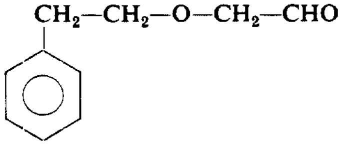
This isomer is not specifically mentioned in the American G.R.A.S. list but it is used in other countries for Pickle flavor compositions (Dill-effect), artificial Pepper oil, etc.

Prod.: by isolation from Waterfennel oil.

26-648; 87-104; 100-790; 160-1150; 163-61; 163-231; B-V-132;

## 2461: PHENETHOXY ACETALDEHYDE

Phenylethyl oxyacetaldehyde.
Do not confuse with: Phenoxyacetaldehyde, see monograph (next).



$C_{10}H_{12}O_2 = 164.21$

Colorless viscous liquid.

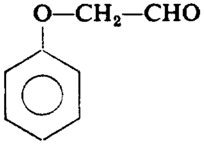
Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-green, tenacious odor.

The title aldehyde is rarely offered under its proper chemical name, but it has been used in perfume compositions for its pleasant sweet, green-floral effect in combination with rosy or jasmin-like materials.

Prod.: various methods, e. g. from Potassium phenylalcoholate and Bromoacetal.

## 2462: PHENOXY ACETALDEHYDE



$C_8H_8O_2 = 136.15$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

The material is relatively unstable and may polymerize if improperly stored, thereby losing odor and increasing its viscosity.

Powerful green, wood-sap-like, but fresh and "aldehydic"-sweet, floral-sweet odor of considerable tenacity. The terminal notes are particularly sweet and attractive.

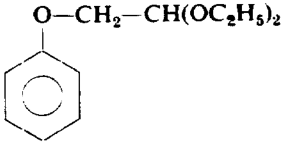
This aldehyde, often .sold under trade names, has found some use in perfume compositions. It performs particularly well with the Ionones and Methylionones for woody-floral complexes, and in Geranium for powerful, fresh-green effects. It can also give lift and novel effects in Lavender with Oakmoss, in Chypre, etc. It is an aldehyde of considerable versatility and power.

Prod.:
1) from Phenol in weak aqueous alkali with Monochloroacetaldehyde dimethylacetal to yield the acetal of the title aldehyde. Oxalic acid hydrolysis affords the aldehyde itself.
2) by hydrolysis of Phenoxyacetylchloride.

The material is unstable unless diluted and refrigerated in storage.

68-428; 163-370;

## 2463: PHENOXYACETALDEHYDE DIETHYLACETAL



$C_{12}H_{18}O_3 = 210.28$

Colorless liquid. B.P. 255° C. Sp.Gr. 1.02.

Insoluble in water, soluble in alcohol and oils.

Mild, green, oily-floral odor of good tenacity.

Some observers claim that the material is odorless when absolutely pure and free from Aldehyde.

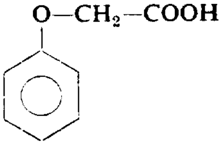
This material has been suggested for use in perfume compositions as a modifier in "green" and green-floral notes, particularly interesting in Lilac and Muguet. However, all indications point at that the material has failed to catch the perfumers' interest, and it is reasonably safe to state that the material is practically obsolete in perfumery.

Prod.: see previous monograph. Monochloroacetaldehyde *diethyl*acetal will afford the title acetal.

28-557; 163-231; 163-370;
The dimethyl acetal is also known, and so is the
*tertiary*-butylacetal(-ethylbutylacetal).
These materials are either extremely rare or actually obsolete in perfumery.

## 2464: PHENOXYACETIC ACID

Phenoxyethanoic acid.
*O*-Phenylglycolic acid.
Phenylium.
Glycolic acid, phenylether.



$C_8H_8O_3 = 152.15$

Colorless needlelike crystals. M.P. 99° C.
B.P. 285° C. (under decomposition).

1.2% soluble in water, soluble in alcohol and oils.

Very faint, acetic-sweet odor of considerable tenacity. The odor is not nearly as cloying as that of Phenylacetic acid, and not as Honey-like, but it is more "sour".

In concentrations below 10 ppm the taste is sweet-honey-like, in higher concentrations slightly sour-fruity. Impure material will show up very clearly on taste, displaying a phenolic off-flavor.

The title acid is a result of chemical research in the field of fungicides and herbicides. Related materials are used as "weed-killers" in the watering of field cultures, while the title acid itself is known as a fungicide. It is not effective as a fungicide in the concentration used in food flavors. .

In imitation Honey, and in various fruit complexes, the acid is used in concentrations equal to 0.3 to 2 ppm in the functional product.

The author has no report of its use in perfumery, but several of its esters are used in fragrance compositions, mainly for Honey-effects, while esters of Phenoxyethanol are used in perfumery for floral effects (see later).

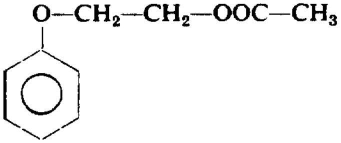
Prod.: from Phenol in aqueous alkali with Monochloroacetic acid.

G.R.A.S. F.E.M.A. No.2872.

26-650; 68-428; 100-798; 160-774; 163-370;
B-VI-161;

## 2465: PHENOXYETHYL ACETATE

Phenylcellosolve acetate.
*2*-Phenoxyethyl acetate.
Ethyleneglycol monomethylether, acetate.



$C_6H_5{-}O{-}CH_2{-}CH_2{-}OOC{-}CH_3$

$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet floral odor of good tenacity.

This ester is not one of the more interesting of the series. It is rarely available commercially, and it does not offer any unique notes, or effects which cannot be obtained from other, readily available, low-cost perfume chemicals.

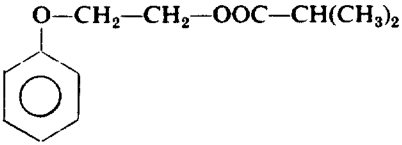
Prod.: by Acetylation of Phenylcellosolve.

163-170;

## 2466: PHENOXYETHYL-iso-BUTYRATE

*2*-Phenoxyethyl-*iso*-butanoate.
"Floranol" (Haarmann & Reimer).
"Phenirat" (Bayer).
Phenylcellosolve-*iso*-butyrate.
Ethyleneglycol monophenylether, *iso*-butyrate.

NOTE: The monograph includes Phenoxyethyl-*n*-butyrate, which is mentioned in literature and normally not distinguished from the title material. Most conceivably, only the *iso*-butyrate has been manufactured for perfumes and flavors, but often labelled "Phenoxyethyl butyrate".



$C_6H_5{-}O{-}CH_2{-}CH_2{-}OOC{-}CH(CH_3)_2$

$C_{12}H_{16}O_3 = 208.26$

Colorless oily liquid. Sp.Gr. 1.05.
B.P. 265° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Sweet-fruity, rosy-floral, slightly honey-like odor of excellent tenacity. Good perfumery grades should show no "metallic" note, generally due to the presence of Glycol-impurities.

The taste at 20 to 50 ppm is sweet-fruity, Peach-honey-like.

This ester has found quite extensive use in perfumery, and it is still surprising to see many perfume laboratories without that material on hand. It has been available from many different suppliers for several decades, it is classified as a comparatively low-cost item, and its odor type should place it among the most frequently used materials for daily use in fragrances for household products, soaps, detergents, room sprays, etc. where "volume" is involved.

It blends excellently with the Ionones and the "rose" alcohols, with Terpineol and Linalool, Hydroxycitronellal and the Nitromusks, in Rose, Sweet Pea, Peony, Lilac, Honeysuckle, etc., and it is stable under normal conditions in various functional products.

The ester finds also use in flavor compositions for imitation fruit flavors, tutti-frutti, etc. partly acting as a fixative.

The concentration used is about 1 to 30 ppm in the finished product.

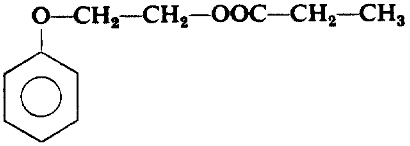
Prod.: by azeotropic esterification of Phenylcellosolve with *iso*-Butyric acid.

G.R.A.S. F.E.M.A. No.2873.

106-284; 163-61; 163-231; 163-373;

## 2467: PHENOXYETHYL PROPIONATE

Phenylcellosolve propionate.
Ethyleneglycolmonophenylether, propionate.



$C_{11}H_{14}O_3 = 194.23$

Colorless oily liquid. B.P. 262° C.

Warm, rosy-fruity, slightly earthy-herbaceous odor of good tenacity. Not as sweet as the *iso*-butyrate, but warmer.

This ester has found some use in perfume compositions, particularly in variations of the Rose theme, where the warm notes from this material are almost inimitable.

Only a few manufacturers offer this chemical, and many perfume laboratories never see it. Which is a shame, because it is truly an interesting chemical with quite unusual effects and a conveniently low cost.

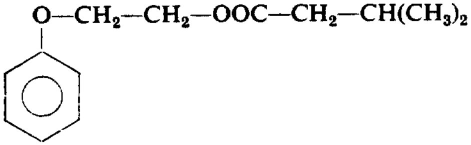
It could find use in many floral types other than Rose, since it blends very well with Cinnamic alcohol, Hydrocinnamic alcohol, Ethyl linalool, etc. and it is stable in soaps and other functional products.

Prod.: from Ethyleneglycol monophenylether and Propionic anhydride.

163-61; 163-231; 163-370;

## 2468: PHENOXYETHYL-iso-VALERATE

Phenylcellosolve-*iso*-valerate.
Ethyleneglycol monophenylether, *iso*-valerate.



$C_{13}H_{18}O_3 = 222.29$

Colorless oily liquid. B.P. 274° C.

Insoluble in water, soluble in alcohol and oils.

Warm-fruity-floral odor of considerable tenacity. The tobacco-like notes seem to replace the honey-notes (in the lower esters), and the fruity theme is discretely Apple-like. The odor is not as herbaceous-fungoid as that of the propionate, but not as warm either.

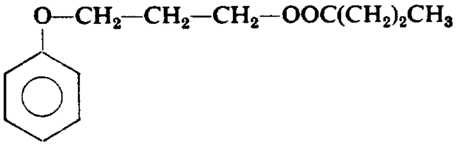
This ester has found some use in perfume compositions as a modifier in Fougères, Chypres, etc., since it blends so well with Oakmoss and Lavender, Coumarin and Amylsalicylate, etc.

It could find use in tobacco flavors, but it is not listed in the American G.R.A.S. list and should therefore not be included in food flavor compositions in the U.S.A.

Prod.: from Ethyleneglycol monomethylether (Phenylcellosolve) with *iso*-Valeric acid by esterification under azeotropic conditions.

## 2469: PHENOXY PROPYL BUTYRATE

*1,3*-Propyleneglycol-monophenylether,*n*-butyrate.



$C_{13}H_{18}O_3 = 222.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, mild-fruity-honey-like, tenacious odor.

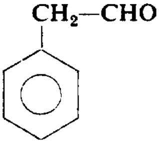
The title ester has been suggested for use in perfume compositions. It was developed after the successful appearance (initially under trade names) of the lower homologue, Phenoxyethyl-*iso*-butyrate.

However, the subject material does not seem to have more or better effects to offer, and it is more expensive than the named lower ester. It is reasonable to believe that the subject material is practically obsolete in perfumery.

Prod.: by esterification of *1,3*-Propyleneglycol-monophenylether with *n*-Butyric acid under azeotropic conditions.

## 2470: PHENYLACETALDEHYDE

*alpha*-Tolualdehyde.
*alpha*-Toluic aldehyde.
*alpha*-Tolyl aldehyde.
*1*-Oxo-*2*-phenylethane.
"Hyacinthin".
"Hyacinth aldehyde".



$C_8H_8O = 120.15$

Colorless liquid. Sp.Gr. 1.03. B.P. 206° C. The pure material may readily form polymers (see below) and it is common practise to store this aldehyde in a 50% solution with Diethyl phthalate to retard such polymerization.

Very slightly soluble in water, soluble in alcohol and oils.

The polymerized material may be practically odorless and the trimer, see below, is a solid material. M.P. 115° C.

Very powerful and penetrating, pungent-green, floral and sweet odor of Hyacinth-type. The tenacity is rather poor, but traces of polymerized material in the commercial product may act as a fixative and give the impression of good tenacity. The odor of such material is naturally weaker.

This aldehyde is widely used in Hyacinth, Lilac, Rose, Lily, Narcisse, Honey, Acacia, Sweet Pea, Cyclamen, Appleblossom (under protest from the author), and countless other fragrance types. In Rose bases it is often accompanied by its Dimethylacetal for emphasis on the earthy-green notes. The normal level of this aldehyde in a perfume oil is 1 to 2%, but it may vary considerably according to type, and to the accompanying materials. The main drawback in the use of this aldehyde is the fact that it is not very stable. Perfumes, made with a conspicuous amount of Phenylacetaldehyde will, after one to three months of storage, show a very perceptible loss of odor power, and the aldehyde may no longer "stand out". The fragrance type changes, and a customer may wonder why his new shipment smells so much "stronger" than his 4-month-old stock of the same perfume. This is bound to happen in almost any perfume in which Phenylacetaldehyde is a conspicuous component.

It is adviseable to use the aldehyde at such (low) concentration that the inevitable change is less perceptible, and also not to keep stock of perfumes in which the aldehyde occurs at relatively high concentration.

Phenylacetaldehyde has a flavor with some resemblance to that of its lower homologue, Benzaldehyde, and it is used to reinforce the effects of Benzaldehyde in Almond and Pistacio imitation flavor. Its sweetness is also utilized in Raspberry, Strawberry, Apricot, Cherry, Peach, Honey and in spice and fruit complexes, etc.

The concentration used is normally very low, about 0.8 to 2 ppm in the finished product, but it may be much higher in chewing gum.

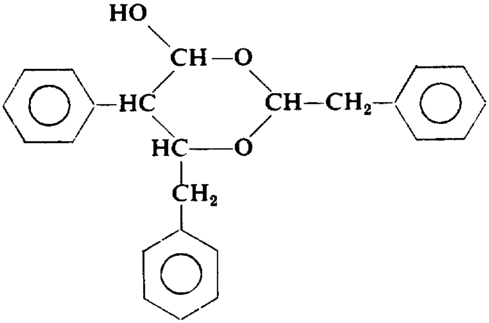
G.R.A.S. F.E.M.A. No.2874.

Prod.: (many methods) e. g. from Styrene oxide, or:
from Cinnamic aldehyde via glycidic ester synthesis.
Also from Benzyl cyanide.
And many other methods.

26-650; 31-38; 31-56; 34-582; 68-527; 89-140; 106-285; 140-161; 160-1248; 163-61; 163-231; 163-370;

NOTE: The published data for Specific Gravity, Boiling Point and even Melting Point (34° C.) for this aldehyde show considerable variations, and it is most conceivable that information has often been based upon impure or partly polymerized material.

The title aldehyde may develop, among other polymers, a trimer of the structure:

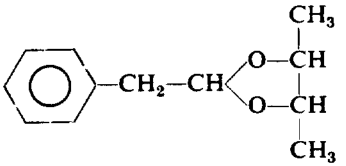


Its chemical name is *2,4*-Dibenzyl-*5*-phenyl-*6*-hydroxy-*1,3*-dioxan, and it is classified as a sesquiacetal of Phenylacetaldehyde with Phenylacetaldol.

The common recommendation that the aldehyde should be diluted with Benzylalcohol (which forms a hemiacetal with the aldehyde) is *not* underwritten by the author, who believes that only a chemically neutral solvent, such as Diethylphthalate can supply a simple dilution of the aldehyde without an incalculable loss in acetalformation.

## 2471: PHENYLACETALDEHYDE-2,3-BUTYLENEGLYCOL ACETAL

*2*-Benzyl-*4,5*-dimethyl-*1,3*-dioxolan.



$C_{12}H_{16}O_2 = 192.26$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-floral, somewhat earthy-fruity odor of good tenacity.

Fruity-fungoid, but rather pleasant taste in concentrations below 10 ppm.

This acetal is used in flavor compositions, mainly in fruit complexes, but also in the rare "floral" flavor type as a fixative/blender.

The concentration is normally as low as 1 to 4 ppm in the finished product.

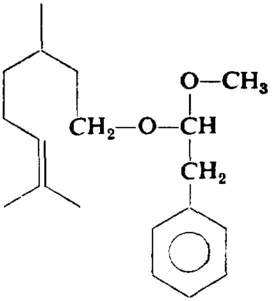
The author has no record of its use in perfume compositions.

G.R.A.S. F.E.M.A. No.2875.

Prod.: by condensation of Phenylacetaldehyde with *2,3*-Butylene glycol.

See also:
Phenylacetaldehyde-*1,2*-dihydroxybutane acetal, and:
Phenylacetaldehyde-*1,3*-dihydroxybutane acetal.

## 2472: PHENYLACETALDEHYDE CITRONELLYL METHYL ACETAL



$C_{19}H_{30}O_2 = 290.45$

Colorless or very pale yellowish oily liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and delicately green-rosy, floral, tenacious odor.

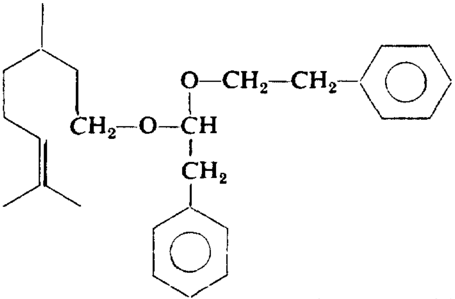
The title "mixed acetal" is briefly mentioned in this work among a considerable number of other acetals of Phenylacetaldehyde as example of the many types in use, or formerly in use.

Most of these "sophisticated" acetals have had a rather short life and little success, while a few have lived a long time, perhaps because they were cleverly incorporated in a specialty and never sold as such under their proper chemical name.

This acetal has found some use in soap perfumes and other perfumes, but is now more or less obsolete in perfumery.

Prod.: by reaction of Phenylacetaldehyde-dimethylacetal with Citronellol.

## 2473: PHENYLACETALDEHYDE CITRONELLYL PHENYLETHYLACETAL



$C_{28}H_{36}O_2 = 404.60$

Colorless viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet and very tenacious, floral-honey-like odor.

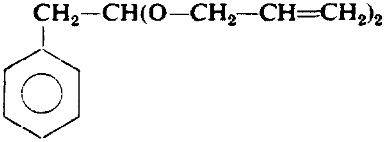
The title acetal is another example of a "sophisticated" combination product of rather disappointing value.

Apparently hoping to achieve an unusual chemical from two well known and successful perfume chemicals (or three materials), this acetal was developed many years ago, but never achieved much popularity.

It is not commonly available and may be considered as practically obsolete in perfumery.

Prod.: by reacting Phenylacetaldehyde diphenylethylacetal with Citronellol. The reaction is presumably incomplete, and the resulting acetal not free from the parent materials.

## 2474: PHENYLACETALDEHYDE DIALLYLACETAL



$C_{14}H_{18}O_2 = 218.30$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Intensive, pungent-green odor, reminiscent of cut grass.

This acetal has been suggested for use in perfume compositions as part of novel top-notes, green notes, etc.

However, the "grassy-green" theme is very well covered as far as natural-smelling raw materials are concerned. Furthermore, there is a general reluctance in using Allyl-derivatives if they present any danger of decomposition in the fragrance.

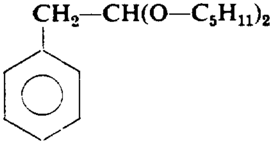
The title acetal would, in fact, present a hazard of decomposition since it may produce trace amounts of Allyl alcohol under mildly acid conditions, which is not uncommon in perfumes.

It is therefore reasonable to assume that the subject acetal has been abandoned and is practically obsolete in perfumery.

Prod.: from Phenylacetaldehyde by condensation with Allyl alcohol.

163-370;

## 2475: PHENYLACETALDEHYDE DIAMYLACETAL



$C_{18}H_{30}O_2 = 278.44$

Colorless liquid. B.P. 245° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

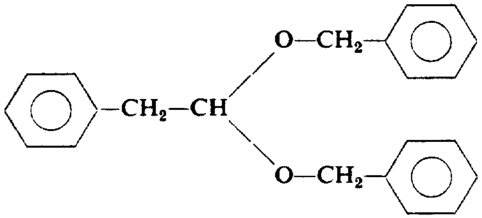
Herbaceous-green, but not very pleasant odor of moderate tenacity.

This acetal does not present the more desirable type of the green odors, but it has found a little use in Hyacinth and Narcisse type fragrances. There is considerable difference in the odor of products from various suppliers, probably because of the type of Amylalcohol used.

Prod.: by condensation of Phenylacetaldehyde with Amylalcohol. Also from Benzylmagnesium chloride and Amyl-*ortho*-formate.

163-61; 163-231; 163-370;

## 2476: PHENYLACETALDEHYDE DIBENZYLACETAL



$C_{22}H_{22}O_2 = 318.42$

Colorless liquid. Sp.Gr. 1.08.

Practically insoluble in water, soluble in alcohol and oils.

Mild, yet rather heavy-floral, sweet and tenacious odor.

This acetal has found some use in perfume compositions for its ability to supply a pleasant, not very conspicuous, green-forest-like and slightly earthy undertone, useful in Muguet and Lilac compositions.

It blends well with the carbinols and the rose alcohols, and it has a mellowing effect upon Indole, often used in such compositions.

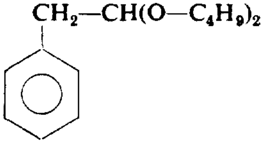
Due to the apparent "weakness" of the material it can be used in concentrations of 10% or more in the perfume oil. It supplies a certain amount of fixation at that level.

Prod.: by condensation of Phenylacetaldehyde with Benzylalcohol.

31-71; 37-512; 43-157; 163-61; 163-232;

## 2477: PHENYLACETALDEHYDE DI-BUTYLACETAL

This monograph includes the *iso*-butylacetal, since the name "butylacetal" in perfumery literature has been used indiscriminately for both.



$C_{16}H_{26}O_2 = 250.38$

Colorless liquid. Sp.Gr. 0.93. B.P. 240° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-floral, delicately green, refreshing odor of good tenacity.

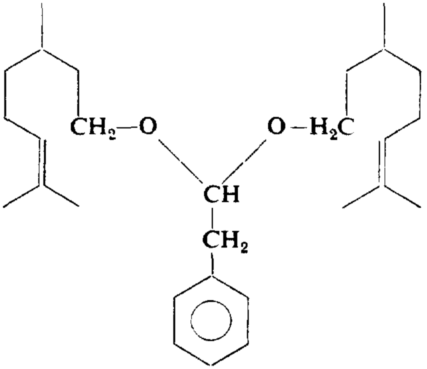
This acetal is used in perfume compositions for its refreshing combination of floral and delicately green notes, blending very well with Cyclamenaldehyde, Lilial, etc. e. g. in Muguet modifications, Peony, Freesia, Appleblossom, etc.

The material is rarely offered under its proper chemical name, but this could be taken as a sort of flattery for the usefulness of that acetal. It is incorporated in certain specialties and occasionally offered under trade names.

Prod.: from Benzyl magnesium chloride and Butyl-*ortho*-formate. Also from Phenylacetaldehyde and Butyl alcohol.

33-158; 163-61; 163-231;

## 2478: PHENYLACETALDEHYDE DICITRONELLYLACETAL



$C_{28}H_{46}O_2 = 414.68$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild and sweet-floral, slightly green and very tenacious odor.

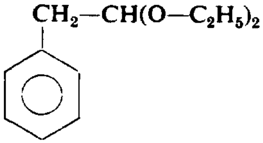
This acetal – and the equivalent Geranylacetal, see later, – represent probably the ultimate in sophistication of Phenylacetaldehyde acetals.

It should be fairly clear to the research chemist now, that successful perfume chemicals are not necessarily created from other, well-established and successful perfume raw materials by calculated combination. And olfactory effects of raw materials may not be doubled, or even duplicated, in a resulting end product.

The title acetal does have a pleasant odor, but considering the amount of trouble one has to go through to achieve this acetal, it is really not worth it. And it is not exaggerated to say that this acetal is practically abandoned and obsolete in today's perfumery.

## 2479: PHENYLACETALDEHYDE DIETHYLACETAL

"Alleglal" (Allondon).



$C_{12}H_{18}O_2 = 194.28$

Colorless liquid. B.P. 245° C. Sp.Gr. 0.96.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-foliage-like, intensively green and moderately tenacious odor. More refined or delicate, less pungent-green than the Dimethylacetal.

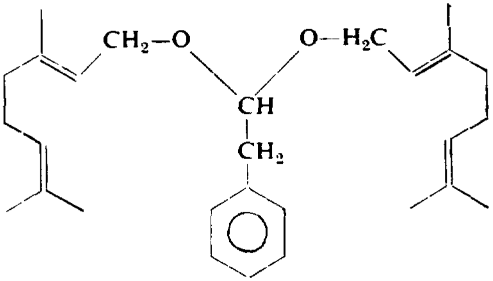
This acetal was for a long time known only under a trade name, and it became quite successful in spite of the free availability of many related materials at that time.

It is still used in perfume compositions where a more discrete green, Lilac-green effect is desirable, and less earthy-gassy notes wanted.

Prod.: from Benzyl magnesium chloride and Ethyl-*ortho*-formate.

5-315; 7-336; 163-61; 163-231; 163-370;

## 2480: PHENYLACETALDEHYDE DIGERANYLACETAL



$C_{28}H_{42}O_2 = 410.64$

Colorless oily liquid.

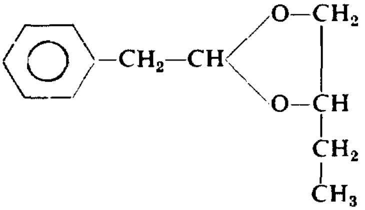
Insoluble in water, soluble in alcohol and oils.

Deep-sweet, heavy and rosy-herbaceous, slightly earthy odor of very good tenacity.

The remarks made about Phenylacetaldehyde di-citronellylacetal (see that monograph, earlier) could be repeated here. The title material does not offer substantial advantages or unique odor type, and it may be considered of little more than academic interest today.

## 2481: PHENYLACETALDEHYDE-1,2-DIHYDROXYBUTANE ACETAL

*5*-Ethyl-*2*-benzyl-*1,3*-dioxolan.



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid.   B.P. 233° C.

Almost insoluble in water, soluble in alcohol and oils.

Earthy-green, pungent floral odor of moderate to poor tenacity.

Although this odor can be classified as a Hyacinth, it has not become very popular. There are similar acetals with Hyacinth type odor, floral, green and earthy, and some of them are superior in performance.

Prod.: by condensation of Phenylacetaldehyde with *1,2*-Butylene glycol.

31-73; 5-323; 163-231;

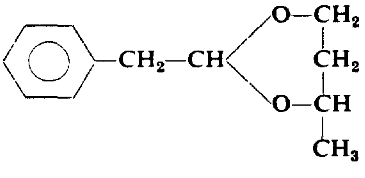
See also:

Phenylacetaldehyde-*2,3*-butylene glycol acetal, and

Phenylacetaldehyde-*1,3*-dihydroxybutane acetal (next).

## 2482: PHENYLACETALDEHYDE-1,3-DIHYDROXYBUTANE ACETAL

*6*-Methyl-*2*-benzyl-*1,3*-dioxan.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Sweet-earthy, green-floral Hyacinth type odor. Not quite as sweet as the odor of the *1,2*-dihydroxybutane acetal.

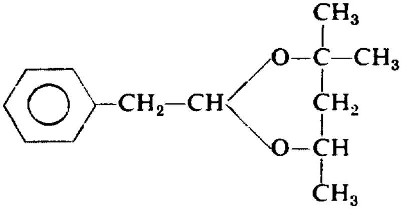
The remarks made about the previous material could be generally repeated here. The subject material has little more than academic interest since it loses out in competition with many superior acetals of this series.

Prod.: by condensation of Phenylacetaldehyde with *1,3*-Dihydroxybutane-(*1,3*-Butylene glycol).

31-73;

## 2483: PHENYLACETALDEHYDE-2,4-DIHYDROXY-4-METHYLPENTANE ACETAL

*4,4,6*-Trimethyl-*2*-benzyl-*1,3*-dioxan.
*2*-Benzyl-*4,4,6*-trimethyl-*meta*-dioxan.



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid. B.P. 242° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-green, warm-earthy odor of moderate tenacity. The green-earthy complex is generally classified as "Reseda"-like, which is highly appreciated in perfumery, although very few perfumers know what Reseda smells like. The peculiar thing about this odor description is, however, that "Reseda"-like normally refers to the odor of the root, not the foliage or the flowers of the Reseda plant, and the root is certainly not an item common to any perfumer's memory.

Nevertheless, the term has become almost synonymous with certain cyclic acetals of Phenylacetaldehyde, and only the Phenylethyl-*iso*-thiocyanate, see monograph, has achieved better fame as a "Reseda" material.

The title acetal finds use in perfume compositions in combination with Oakmoss and Vetiver, with Lavender and Rose materials, etc. or in special "green" bases, specialties, etc.

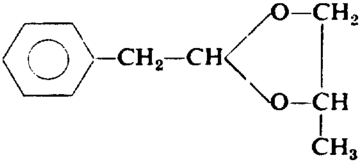
It is not always sold under its proper chemical name, since many specialties are based upon this or related acetals, and sold under confusing trade names.

Prod.: from Trimethyl-trimethyleneglycol (= *4*-Methylpentane-*2,4*-diol) plus Phenylacetaldehyde by condensation.

5-323; 31-73; 163-232;

## 2484: PHENYLACETALDEHYDE-1,2-DIHYDROXYPROPANE ACETAL

Phenylacetaldehyde propylene glycol acetal.
*5*-Methyl-*2*-benzyl-*1,3*-dioxolan.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid. B.P. 229° C.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-rosy, floral and sweet-green odor of moderate to poor tenacity.

This acetal is used in perfume compositions as a modifier, not only for rose compositions, but in many floral types, woody bases, Chypre types, Fougères, etc.

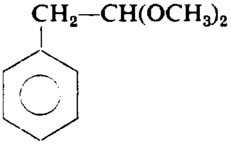
It blends very well with Cinnamic alcohol, Styrax, the Eugenols, rose alcohols, Linalool and esters, etc. but it needs considerable fixation to perform satisfactorily.

Prod.: by condensation of Phenylacetaldehyde with Propylene glycol.

5-323; 31-73; 163-62; 163-232;

## 2485: PHENYLACETALDEHYDE DIMETHYLACETAL

"P.A.D.M.A.".
*alpha*-Tolylaldehyde dimethylacetal.
*1,1*-Dimethoxy-*2*-phenylethane.
"Vertodor".
"Viridine" (Givaudan).
"Vert de Lilas".
"Gladioline".
"Vertifol". (part-component).
"Jacinthal".
"Foliol Rosal".
"Foliacetal".
"Hyacylene".
"Rosal",
- and many other trade names. The title material constitutes all or the major part of the named "specialties" under trade name.



$C_{10}H_{14}O_2 = 166.22$

Colorless liquid. Sp.Gr. 1.01. B.P. 221° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful green-earthy, flower-stem-like odor, not as pungent as that of the aldehyde, and without the "Bitter-almond" note of Phenylacetaldehyde.

At concentrations below 10 ppm the taste is sweet-green, honey-spicy, but at higher concentrations it tends to be bitter, unpleasant.

This is one of the most widely used "acetals" in perfumery. Although always a minor component, it enters a multitude of fragrance types where it may lend green notes, earthy notes, floral notes, spicy notes or simply power. It performs excellently with Oakmoss and Vetiver, Geranium, Opopanax, etc. in Lilac, Rose, Muguet, Oriental bases, etc. and with the Methylionones in woody-floral-spicy complexes. It is often used in Gardenia, Reseda and Carnation to lend spicy foliage note to the sweet florals, or earthy-rooty notes in Reseda.

The acetal finds some use in flavor compositions for imitation Apricot, Cherry, Honey, spice and fruit-blends, etc. but the concentration is usually as low as 0.5 to 10 ppm in the finished product.

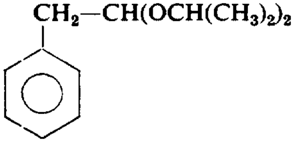
G.R.A.S. F.E.M.A. No.2876.

Prod.: from Phenylacetaldehyde and Methanol with dry Hydrogen chloride as dehydrating agent.

5-315; 33-158; 106-286; 140-161; 163-232; 163-62; 103-284; 156-299;

## 2486: PHENYLACETALDEHYDE DI-iso-PROPYLACETAL

Sometimes called:
Phenylacetaldehyde di-propylacetal.



$C_{14}H_{22}O_2 = 222.33$

Colorless mobile liquid. B.P. 230° C. Sp.Gr. 0.95.

Practically insoluble in water, soluble in alcohol and oils.

Slightly musty, green-herbaceous odor of moderate to poor tenacity.

This acetal has been suggested for use in perfume compositions, but its odor type and overall character leaves much to be desired or, in other words, it is not sufficiently interesting and different from the many other acetals available.

Much more interesting is the "mixed" acetal of Phenylethyl alcohol and Propyl alcohol upon Acetaldehyde, see monograph:

Acetaldehyde phenylethyl-*n*-propylacetal (Acetal R).

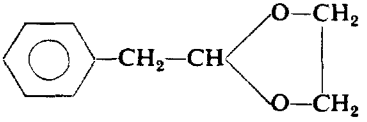
The title material can justly be classified as practically obsolete and of little more than academic interest to perfumery.

Prod.: from Benzyl magnesium chloride and (*iso*)Propyl-*ortho*-formate.

163-62; 163-232;

## 2487: PHENYLACETALDEHYDE ETHYLENEGLYCOL ACETAL

*2*-Benzyl-*1*,*3*-dioxolan.
Phenylacetaldehyde ethylene acetal.



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid. Sp.Gr. 1.05.

Practically insoluble in water, soluble in alcohol and oils.

Clean and mild, fresh-rosy, leafy odor of moderate to poor tenacity.

This acetal has been in use in perfumery for a long time, and it is well liked by some perfumers, while many others cannot see any effect in it.

It is true that the effect is only perceptible in-use. The material itself, when pure, does not impress the observer the first time he smells it. But it has an overall refreshing effect upon floral and floral-green fragrance types.

For Hyacinth, Rose, Narcisse, Muguet, etc. it finds use at relatively high concentration, often in combination with the carbinols, supporting the floral greenness of those materials.

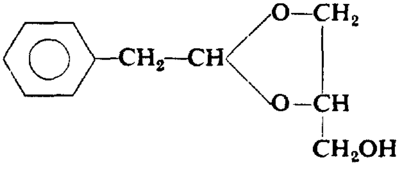
It is interesting to compare the structure and odor of this material to Formaldehyde phenylethyleneglycol acetal (*4*-Phenyl-*1*,*3*-dioxolan) see that monograph (1409).

Prod.: by condensation of Phenylacetaldehyde and Ethyleneglycol.

31-73; 43-158; 84-1; 163-61; 163-231;

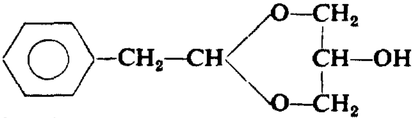
## 2488: PHENYLACETALDEHYDE GLYCERYLACETAL

The commercial product consists of a mixture of the two acetals:
I: *5*-Hydroxymethyl-*2*-benzyl-*1*,*3*-dioxolan.
II: *5*-Hydroxy-*2*-benzyl-*1*,*3*-dioxan.



I: about 60% of commercial prod.

and:



II: about 40%.

$C_{11}H_{14}O_3 = 194.23$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very faint, sweet-green, rosy odor with peculiar semi-dry undertones. Moderate to good tenacity.

Sweet and mildly green taste in concentrations below 20 ppm, but tends to become "perfumey" at higher levels.

This acetal – like the previously mentioned – does not impress the observer on the first encounter, but it has very pleasant effects when used in sufficiently high concentration in Rose, Chypre, Hyacinth, Lilac, etc. as an "undertone" material. It is excellent for "forest"-green undertones in Muguet, or for the deep-green leafy notes of Lilac, but it needs supporting notes, and it is not a powerful odorant.

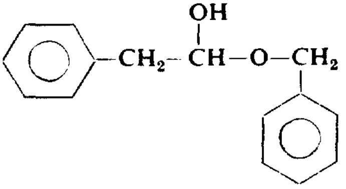
The subject acetal is also used in flavor compositions as a fixative in certain fruit types, and in "floral" flavor types as a bouquetting material in traces. The concentration used is about 5 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2877.

Prod.: from Phenylacetaldehyde and Glycerol by condensation.

5-322;

## 2489: PHENYLACETALDEHYDE MONOBENZYLACETAL



$C_{15}H_{16}O_2 = 228.29$

Colorless viscous liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Slightly green-woody, very mild and delicate odor of moderate tenacity.

The title hemiacetal is briefly mentioned in this work because it may occur as component in stock containers of Phenylacetaldehyde 50% – if the dilution has been made with Benzylalcohol. This has been common practice, but the author believes that Benzylalcohol as a diluent has been largely abandoned today.

Phenylethylalcohol has also been used, but it will, although to a lesser degree, form hemiacetal with Phenylacetaldehyde upon storage in 50/50 solution.

The reaction may take place gradually, and the speed of progress depends upon temperature, daylight and other conditions.

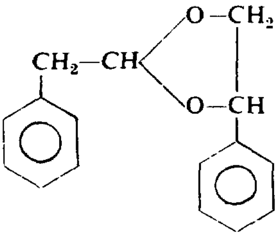
It is therefore reasonably safe to say that the title material has only little more than academic interest, and it is an ill-defined material unless intentionally prepared in a laboratory.

Prod.: by condensation of equimolecular proportions of Benzylalcohol and Phenylacetaldehyde.

31-71;

## 2490: PHENYLACETALDEHYDE PHENYLETHYLENEGLYCOL ACETAL

*4*-Phenyl-*2*-benzyl-*1,3*-dioxolan.



$C_{16}H_{16}O_2 = 240.30$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar oily-green, earthy-rooty, but mild and sweet odor of good tenacity.

This acetal has been suggested for use in perfume compositions as a "Reseda"-acetal for its sweet-earthy-green notes, but it does not seem to have achieved the same popularity as many of the other Phenylacetaldehyde-(cyclic)-acetals.

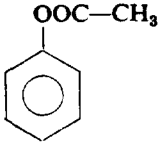
The immediate impression is that the material has very little odor at all, but once it is incorporated in a composition including more volatile components, the true character of the subject acetal is brought about in a more conspicuous way.

It can bring very pleasant nuances into a Muguet, or a natural background note in Lilac. It gives interesting notes with Lavender and Opopanax, Amylsalicylate, etc. in Fougère, and warm-spicy undertones in a Rose fragrance.

Prod.: by condensation of Phenylacetaldehyde and Phenylethyleneglycol.

## 2491: PHENYL ACETATE

Acetyl phenol.



$C_8H_8O_2 = 136.15$

Colorless liquid. Sp.Gr. 1.08. B.P. 196° C.

0.03% soluble in water, miscible with alcohol and oils.

Floral, but somewhat harsh odor of Lily-Jasmin type. Impure products may show phenolic notes, while a "metallic" note seems to be normal in this material.

The title material has been suggested for use in fragrances, but the author is of the impression that this material has not been in common use in perfumery for many decades. It dates back to the very early days of synthetic perfume chemicals, and it has been outperformed by many newer chemicals in use today.

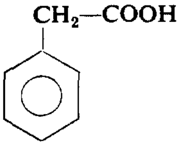
It is physically interesting, because its refractive index is almost identical to that of common flint glass. Which means that it is almost "invisible" in a glass container.

Prod.: by acetylation of Phenol with Acetylchloride and aqueous alkali in the cold.

26-652; 68-431; 100-799; 160-1152; 163-232; B-VI-152;

## 2492: PHENYLACETIC ACID

*alpha*-Toluic acid.



$C_8H_8O_2 = 136.15$

White leafy crystals. M.P. 77° C.
B.P. 266° C. Sp.Gr. 1.08 (liquid).

2% soluble in cold water, better in hot water. Soluble in Propylene glycol, miscible with alcohol and oils.

Sweet, animal-honey-like odor of extraordinary tenacity. The sweet-honey-like character is predominant at very low concentration, while the animal-Civet-like notes appear at higher concentrations.

In aqueous dilution the taste is, like the odor, quite pleasant at extremely low concentrations, e. g. less than 1 ppm, while the more pronounced honey-like notes dominate the taste impression at higher levels.

This acid is one of the most important perfumery acids, and it is widely used, although only in minute proportions, in fragrances and flavors.

With Indole it forms basis of many Civet compositions, and it finds use as part of the fixative base in many floral and Oriental fragrance types: Mimosa, Cassie, Lilac, Jasmin, Neroli, Rose, Carnation, Honeysuckle, Orchid, etc.

Its fixative effect is often underestimated, and unpleasant or undesirable terminal notes may appear in a fragrance, particularly in presence of high-boiling Butyrates and *iso*-butyrates. The title material is, in the author's experience, one of the most tenacious odorants of all known and used perfumery materials. It will outlast Vanillin on a "blotter test" and a 5% solution of Phenylacetic acid may last more than 3 years on a blotter under normal laboratory air-room conditions. Tiny crystal scales of the acid will emanate a very perceptible odor virtually through several decades if left in the open (e. g. embedded in a laboratory tabletop, etc.).

The acid is used in flavor compositions for its Honey-effect (high level) or as a sweetener (very low level), e. g. Butter, Chocolate, Honey, Peach, Rose, Strawberry, Vanilla, etc.

The concentration used may vary from 0.1 ppm to 30 ppm in the finished product.

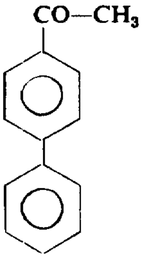
G.R.A.S. F.E.M.A. No.2878.

Prod.: from Benzyl chloride via Benzylcyanide and by acid hydrolysis to the title material. Other methods are known and used.

26-652; 34-582; 68-595; 100-799; 106-289; 160-1256; 140-150; 163-63; 163-233; B-IX-431; 85-98;

## 2493: PHENYL ACETYL BENZOL

Acetyl biphenyl.
*para*-Phenyl acetophenone.
Methyl diphenylketone.



$C_{14}H_{12}O = 196.25$

Prismatic crystals. M.P. 121° C.
B.P. 327° C.

Insoluble in water, soluble in alcohol and oils.

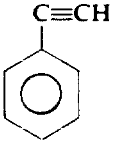
Faint, balsamic odor of excellent tenacity.

This ketone has been used in perfume compositions as an auxiliary fixative, a modifier for Benzophenone or Methyl diphenylether, and as a background note in low-cost Geranium type odors, etc.

It has very little to offer, and its overall odor type does not place it in a class of highly desirable chemicals. Very few perfume laboratories have this material at hand, and the others probably do not miss it much.

26-652; 163-62; B-VII-443;

## 2494: PHENYL ACETYLENE



$C_8H_6 = 102.14$

Colorless liquid. Sp.Gr. 0.93. B.P. 143° C.

Insoluble in water, soluble in alcohol and oils.

Very faint "metallic"-sweet odor. Technical grade material may carry various (conventional and unpleasantly smelling) impurities, typical of Acetylenes.

This material is briefly mentioned because it has been suggested as a perfume chemical, and because it serves as intermediate in the making of several very common fragrance chemicals. It may therefore appear as an impurity in impure grades of such perfume chemicals.

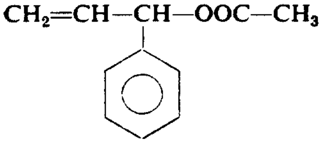
Acetophenone, among other materials, is sometimes made via the title material.

Prod.:
1) from *beta*-Chlorostyrene with alkali.
2) from Acetophenone dichloride with alcoholic Potassium hydroxide at 130° C.
3) from Styrene dibromide with alcoholic Potassium hydroxide.

26-652; 31-6; 68-963; B-V-511;

## 2495: alpha-PHENYL ALLYL ACETATE

Phenyl vinyl carbinyl acetate.
Vinyl phenyl carbinyl acetate.
"*iso*-Cinnamyl acetate".
"*iso*-Styrone acetate".
*1*-Phenyl-*2*-propen-*1*-yl acetate.



$C_{11}H_{12}O_2 = 176.22$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and fruity-honey-like, relatively tenacious odor with discrete balsamic-floral character.

Very sweet, deep-fruity taste with a faintly honey-like character in concentrations below 20 ppm.

This ester is very rarely offered under its proper chemical name, but it has been known to the perfume chemist for several decades.

It has also been available as a major component of various perfume bases, mostly of fruity type.

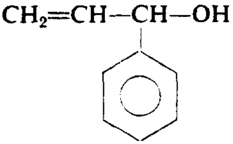
The title ester blends very well with the Ionones, Phenylethylalcohol, Nerol, Hydroxy phenyl butanone, Mimosa, Anisic esters, etc. for Raspberry type fragrances for various cosmetic purposes. It is also useful as a modifier in Honey bases ("miel") with Phenylethylphenylacetate, Styryl esters, etc.

Prod.: by azeotropic esterification of *alpha*-Phenyl allyl alcohol (see next monograph).

See also: Phenyl vinyl acetate.

## 2496: alpha-PHENYL ALLYLALCOHOL

Phenyl vinyl carbinol.
Vinyl phenyl carbinol.
*1*-Phenyl-*2*-propen-*1*-ol.
The material has sometimes been referred to as:
*iso*-Cinnamic alcohol or "*iso*-Styrone".
It exists in *dextro*- and *laevo*-forms.



$C_8H_{10}O = 134.18$

Colorless, slightly viscous liquid.
B.P. 220° C.

Almost insoluble in water, soluble in alcohol and oils.

Warm, spicy-floral and balsamic odor, reminiscent of Phenylethylalcohol and Phenylpropylalcohol at the same time, but overall stronger, heavier, more pungent. Certain qualities of this material appear more floral and more refined than Cinnamic alcohol.

This alcohol is rarely offered under its proper chemical name, but it has been sold under various trade names, and it has been incorporated in certain perfume specialties for several decades.

Yet, in our days of secret-revealing analytical instruments, it has not become truly popular at any time, except for "captive" use by private manufacturers.

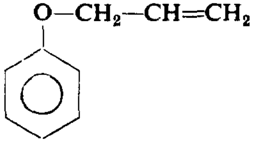
The alcohol performs well in soap, and blends excellently with Cinnamic alcohol as a modifier, with Terpineol or Linalool, Phenylethylalcohol and Amylsalicylate, and with Cyclohexanol derivatives.

Prod.: from Phenylmagnesium bromide plus Acrolein.

68-981; 163-370;

## 2497: PHENYL ALLYL ETHER

Allyl phenyl ether.



$C_9H_{10}O = 134.18$

Colorless liquid. Sp.Gr. 0.98. B.P. 192° C.

Insoluble in water, soluble in alcohol and oils.

Ethereal-rosy, green, slightly "gassy", Geranium-type odor of poor tenacity.

This ether has been suggested for use in perfume compositions for its "Geranium" effect. However, there are many such materials available, and most of them have distinct advantages over the title material.

Better tenacity, better stability, lower cost, etc. are virtues found in a number of other, well known materials with similar odor type.

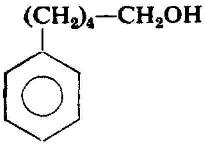
Besides, there has been an increasing reluctance in the use of Allyl-benzenoid compounds, at least until solid proof of absolute harmlessness to human skin is brought out in public.

Prod.: from Phenol and Allyl bromide in Acetone, by heating in the presence of Potassium carbonate.

26-396; 68-426; B-VI-144;
The title material also serves as an intermediate in the manufacture of *ortho*-Chavicol.

## 2498: PHENYL AMYL ALCOHOL

*5*-Phenyl pentanol-*1*.



$C_{11}H_{16}O = 164.25$

Colorless liquid. B.P. 244° C.

Almost insoluble in water, soluble in alcohol and oils.

Light and sweet-herbaceous odor with discretely citrusy-lemony notes, overall resembling Verbena, although not nearly as "lemony".

This alcohol has been recommended for use in perfume compositions, but it has rarely been offered under its proper chemical name. It was once used in perfume specialties under trade name, but the author believes that it is no longer in use of any significance.

It is interesting, however, to notice the rare case of a chemical with a Verbena-type odor, particularly since Verbena has had an unquestionable "come-back" in modern perfumery.

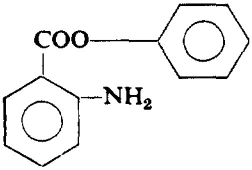
Prod.:

1) from Benzaldehyde by condensation with Butyraldehyde, followed by complete hydrogenation and reduction of the unsaturated aldehyde.
2) from Phenyl magnesium chloride and Ethylene oxide.
3) by reduction of Phenylpentenoic acid, ethylester.

31-23; 7-337; 163-232; 5-58;

## 2499: PHENYL ANTHRANILATE

Phenyl-*2*-aminobenzoate.



$C_{13}H_{11}NO_2 = 213.24$

White or pale straw-colored crystals.
M.P. 70° C.

Insoluble in water, poorly soluble in cold alcohol, soluble in most perfume oils.

Very faint, sweet-floral odor of Orange-blossom-Honeysuckle type.

Very good tenacity. However, a purified, recrystallized material is virtually odorless to most people.

The ester, made by the "old-fashioned" method, actually contained large amounts of odorous, lower ester, and the odor of the title material has forever been described in literature based upon that type material.

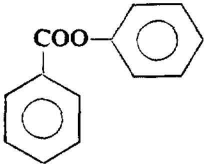
Apart from some unquestionable effect as a fixative, this ester has no interest to the perfumer.

It is very conceivable, that confusion with Phenylethyl anthranilate occurs. The latter material has some application in perfumery, and it is fairly common in the laboratories.

Prod.: from Phenol and Isatoic anhydride.

163-232;

## 2500: PHENYL BENZOATE



$C_{13}H_{10}O_2 = 198.22$

Colorless prismatic crystals. M.P. 70° C.
B.P. 314° C. Sp.Gr. 1.23 (liquid).

Very slightly soluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and oils.

Very faint, balsamic-floral, metallic-green odor of excellent tenacity.

This material could serve as a fixative in perfume compositions, but it does not present any advantage over the conventional crystalline fixatives of similar odor type.

Since the material presents some hazard of producing a phenol in decomposition under alkaline conditions, it can not be recommended in modern perfumery.

There is a possibility of confusing the name of the title material with that of Phenylethyl benzoate, which is more odorous and more frequently found on the perfumer's shelf.

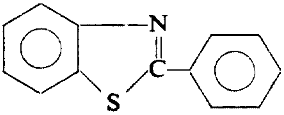
The subject material could be considered as practically obsolete in modern perfumery.

Prod.: from Phenolsodium and Benzoylchloride.

26-652; 100-800; 160-850; 163-63; B-IX-116;

## 2501: 2-PHENYL BENZOTHIAZOLE

*2*-Phenyl-(*1,3*-benzthiazole).
Benzenyl-*ortho*-aminothiophenol.



$C_{13}H_9NS = 211.29$

White crystalline powder. M.P. 115° C.
B.P. 360° C.

Insoluble in water, poorly soluble in alcohol, soluble in some, but not all, perfume oils.

Very mild, green-rosy, slightly metallic odor, in solution developing a pleasant, sweet-tea-rosy odor type. Good tenacity.

This is another material which is more often described and talked about than actually used in the perfume laboratory.

Even the few well equipped laboratories who have this material on shelf, may probably not use it ever, or just try it once or twice. It is rather disappointing, particularly after reading so much and so often in literature about it.

The author would dare classify the material as obsolete and absolutely dispensable in perfumery.

It has occasionally been used as a fixative in woody-rosy Geranium type fragrances, etc., and it has been known for about half a century in the perfume laboratory. It was one of the first sulfur-compounds to be honored with a space on the perfumer's shelf.

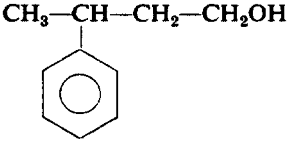
Today, we have quite a number of sulfur-compounds of altogether different composition at hand for delicate work in creative perfumery and reconstruction of essential oils, etc.

Prod.:
1) from *ortho*-Aminothiophenol and Benzoyl chloride.
2) from Benzylaniline plus Sulfur.

69-427; 95-205; 163-371; 31-200; 159-433;

## 2502: 3-PHENYL-1-BUTANOL

*3*-Methyl-*3*-phenylpropanol-*1*.
This material is often called "Phenyl butyl alcohol", and it can therefore be confused with *4*-Phenylbutanol-*1*, which is described in this work under the proper name:
Phenyl butyl alcohol.
The two materials are isomers.



$CH_3-CH(C_6H_5)-CH_2-CH_2OH$

$C_{10}H_{14}O = 150.22$

Colorless, slightly viscous liquid.
B.P. 231° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Warm and relatively powerful balsamic-rosy odor of moderate tenacity.

This alcohol has been used as a modifier for Phenylethyl alcohol in Rose compositions and, in general, as a floral and warm, versatile component for Oriental, woody, floral and balsamic fragrance types. It is considered as a stronger version of Phenylethyl alcohol, but the perfumer would do more justice to this material if he regarded it as an independent material, not a substitute.

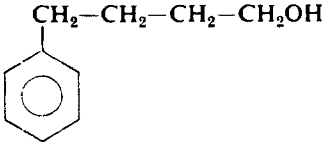
Newer carbinols have partly taken over much of the space previously filled by this and similar materials, because the carbinols generally possess greater strength and tenacity. However, the title material remains in use in a number of specialties and successful bases.

Prod.: by reduction of the Methylester of *3*-Phenylbutyric acid.

5-57;
see also: Phenyl butyl alcohol.

## 2503: PHENYL BUTYL ALCOHOL

*gamma*-Phenyl-*n*-butylalcohol.
*4*-Phenylbutanol-*1*.



$C_{10}H_{14}O = 150.22$

Colorless oily liquid. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, but rather heavy, herbaceous-rosy odor, heavier and less rosy than Phenylethyl-alcohol, but more tenacious.

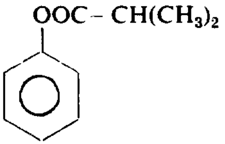
The title alcohol has, on account of its faintly woody-green floral character, found use in perfume compositions as part of the base for Mimosa and Cassie compositions, Rose bases, Oriental fragrance types, etc.

In view of the scarcity of materials suitable for Mimosa type odors, it is interesting to note that this material is rarely, if ever, mentioned or offered commercially. The corresponding aldehyde is somewhat better known (see monograph later) (2506).

Prod.:
1) from Phenylacetaldehyde and Acetaldehyde by condensation, followed by hydrogenation and reduction of the unsaturated aldehyde.
2) from Phenylethyl magnesiumbromide plus Ethylene oxide in a Grignard type reaction.

31-23; 68-501; 163-233; 163-371;
(see also: *3*-Phenyl-*1*-butanol).

## 2504: PHENYL-iso-BUTYRATE



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Pungent-heavy, Honey-fruity odor with distinctly animal undertones.

The odor of this material is heavily influenced by the presence of traces of free Phenol or free Butyric acid.

However, the main – or perhaps only – field of application for this material is in artificial Civet compositions, or perhaps in certain very heavy, exotic type florals.

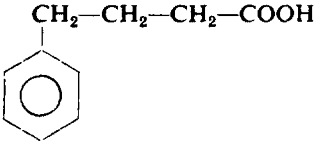
The tenacity is very good, but the odor type difficult to control, and the material is simply not very popular or commonly used.

It is very conceivable that confusion with the name of the much more common perfume chemical, Phenylethyl-*iso*-butyrate, occurs.

Prod.: from Phenol in cold aqueous alkaline solution with *iso*-Butyric anhydride.

## 2505: PHENYL BUTYRIC ACID

*4*-Phenylbutanoic acid.



$C_{10}H_{12}O_2 = 164.21$

White crystals. M.P. 52° C.

Almost insoluble in water, soluble in alcohol and oils.

Very faint, but very tenacious, sweet-heavy, floral-honey-like odor. The crystals may carry an odor of quite different character, since they easily absorb odor from surrounding perfume materials. But in solution, the heavy sweetness becomes more obvious, and traces of contamination may be eliminated.

The title acid has been suggested for use in perfume compositions, partly as component of artificial Civet, partly in certain heavy floral bases. Derivatives of the acid are more commonly used.

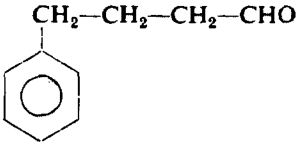
Prod.:

1) by acid hydrolysis of Phenyl propyl cyanide.
2) by reduction of Phenyl butyrolactone.
3) from Phenyl-*n*-propylketone and yellow Ammonium sulfide.
4) from Benzoylpropionic acid by Clemmensen's reduction.

68-597;

## 2506: PHENYLBUTYRIC ALDEHYDE

Phenyl butyraldehyde.
*gamma*-Phenyl-*n*-butanal.
*4*-Phenylbutanal.



$C_{10}H_{12}O = 148.21$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, fruity-floral and sweet, tenacious odor.

The fruity notes resemble Peach and Mango, while the floral tones are mainly rosy.

This aldehyde has been used in perfume compositions under various trade names and has rarely been offered under its proper chemical name.

It does not seem to be highly interesting and apart from occasional "captive" use of this aldehyde, it may slowly disappear from the perfumery shelves again, if it ever were there.

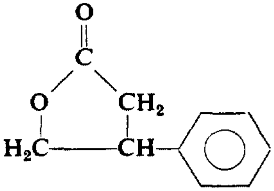
Its use in certain rose bases probably made analytical perfume chemists believe that it was a "key" material, but experiments show that it is not indispensable.

Prod.: by oxidation (more correctly called dehydrogenation) of *4*-Phenylbutan-*1*-ol (see previous monograph).

163-63;

## 2507: PHENYLBUTYROLACTONE

*gamma*-Phenyl-*gamma*-butyrolactone.
Although literature includes reference to the isomer, *alpha*-Phenyl-*gamma*-butyrolactone and suggests its use in perfumery, the author believes that the *gamma*-substituted Lactone is the most commonly used of the two.



$C_{10}H_{10}O_2 = 162.19$

White crystalline mass, opaque mass, or supercooled, viscous liquid. The solid material melts at 38° C.

Practically insoluble in water, soluble in alcohol and oils.

Very mild, faintly-balsamic, creamy and tenacious odor.

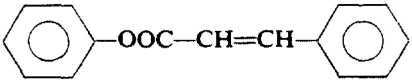
This rare lactone is used occasionally in perfume compositions as supporting note in sweet-woody and balsamic-Oriental fragrance types. It blends very well with Ylang-Ylang, Methylionones, Benzoin, Sandalwood and Labdanum for those types, but it does not contribute much odor power to the composition.

Prod.: from Phenylethylene oxide and Sodiomalonic ester.

31-170; 163-233; 163-371; 159-418; 159-421; The literature references include those mentioning the *alpha*-substituted lactone.

## 2508: PHENYL CINNAMATE

The title material could be confused with the isomer: *trans-alpha-beta*-Diphenylacrylic acid, which is *alpha*-Phenylcinnamic acid.
The author also suspects occasional confusion with the more commonly used perfume chemical: Phenylethyl cinnamate (see monograph).



$C_{15}H_{12}O_2 = 224.26$

White crystals.

Insoluble in water, soluble in alcohol and oils. The solubility in alcohol is poor, but sufficient for normal perfume compounding.

Very faint, sweet, floral-balsamic odor. Aged or impure material may carry undesirable phenolic notes.

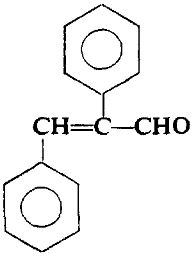
This material has been used in perfume compositions as a fixative in balsamic and Oriental fragrance types, but the author believes that the use of this item is practically abandoned. Its contribution to the odor of a composition is minimal, and its fixative effect easily duplicated with more modern and stable materials.

The fact that decomposition may create phenolic odor is another reason not to use the title material.

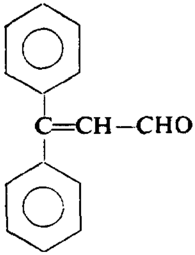
Prod.: from Phenolsodium and Cinnamoylchloride.

68-432;

## 2509: PHENYLCINNAMIC ALDEHYDE



*alpha*-Phenylcinnamic aldehyde



*beta*-

$C_{15}H_{12}O = 208.26$

Pale yellowish viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Very faint, sweet, oily-balsamic odor of considerable tenacity.

Since it is the author's impression that the title material is obsolete, the mention is mainly aimed at elucidating the rather complicated information and incomplete data given in the scarce literature sources.

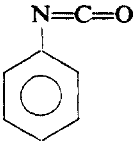
The *alpha*-Phenylcinnamic aldehyde could be prepared from Benzaldehyde by condensation with Phenylacetaldehyde, but the reaction may well produce polymers of Phenylacetaldehyde which are odorless and useless in perfumery. See monograph on Phenylacetaldehyde.

The *beta*-Phenylcinnamic aldehyde is known, but not likely to be suggested for perfumes.

31-52;
see also report in: Der Seifensiederzeitung (1935), vol. 62, pages 171-172.

## 2510: PHENYL-iso-CYANATE

Phenylcarbimide.
Carbanil.
Phenylcarbonimide.



$C_7H_5NO = 119.13$

Colorless mobile liquid. Sp.Gr. 1.10.
B.P. 162° C.

Decomposes in water and alcohol, soluble in oils.

Extremely penetrating, repulsive and irritating odor when undiluted. "Soapy"-sweet odor in extreme dilution. Although it cannot be classified as tenacious, the odor is persistent and annoying in minute traces.

This material is not a perfume material but it is included in this work to elucidate a possible problem of hazardous confusion with Phenylethyl-*iso*-thiocyanate (Phenylethyl mustard oil) which is used in flavors.

The title material is a relatively mild lachrymator and classified as a "discomfort gas". It is simply unpleasant to be exposed to the odor and the material has found use for exactly that purpose: to dispense prior to the use of a poison gas, so that the use of a gas mask becomes unbearable on account of sneezing and coughing.

Numerous chemicals, closely related to perfume and flavor materials may have similar effects, but the literature covers the subject very comprehensively.

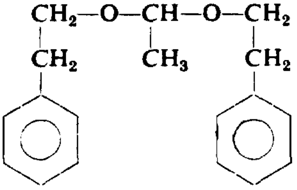
Prod.:

1) from Phosgene in hot Aniline with Hydrogen chloride.
2) from Chloroform and Aniline, by oxidation.

26-654; 68-201; 100-804; 163-372; B-XII-437; (Private experiments).
See also monograph: Phenylethyl-*iso*-thiocyanate.

## 2511: PHENYLETHYL ACETAL

Acetaldehyde di-phenylethylacetal.
Do not confuse with Phenylethyl acetate.



$C_{18}H_{22}O_2 = 270.37$

Colorless liquid. Sp.Gr. 1.02.

Very slightly soluble in water, miscible with alcohol and oils, soluble in Propylene glycol.

Warm, green-leafy, also rosy-balsamic and rich, tenacious odor. Sweet-green taste in concentrations below 10 ppm.

The odor has occasionally been described as "horseradish-like", but the author believes that this description must refer to another material.

The title acetal is one of the more successful acetals, since it definitely has an odor of its own, a good stability, and versatility in perfume creation. It finds use in Gardenia, Hyacinth, Lilac, Rose, Oriental, Carnation, Muguet, etc. and often as part of a topnote complex with or without the Hexenyl esters, etc.

Its leafy character is pleasantly subdued by warm, balsamic-rosy notes, and it is in no way pungent, although it could be classified as moderately powerful. It blends extremely well with Galbanum.

It would normally be used at concentrations near one percent in a perfume oil, rarely higher than 3%.

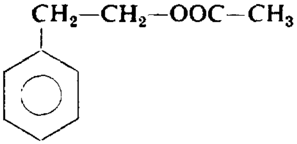
The material is used in flavor compositions for fruity green effects in Blackcurrant, Cucumber, Apple, etc. except in the U.S.A. since it is not included in the American G.R.A.S. list.

Prod.: from Phenylethylalcohol and Acetylene.

31-65; 106-291; 140-157; 163-62;

## 2512: PHENYLETHYL ACETATE

*beta*-Phenethylacetate.
*2*-Phenylethyl acetate.
Benzyl carbinyl acetate.



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid. Sp.Gr. 1.05.
B.P. 232° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Very sweet, rosy-fruity, honey-like odor of moderate to poor tenacity. The fruity notes are mostly peachy with a pleasant leafy-green tonality, the rosy notes very sweet, almost towards Gardenia. Variations in the odor of this material will naturally follow the pattern of the parent alcohol in which sharper, more pungent notes are typical of the commercial grades, while warm, deep-rosy notes with balsamic softness are typical of the highly refined grades.

The taste at concentrations below 10 ppm is sweet, fruity-honey-like, remotely Raspberry-like, but at higher levels rather "perfumey" not quite attractive.

The title ester is widely used in perfume compositions, from everyday soap and detergent perfumes to fine cosmetic fragrances, room-sprays, deodorants, etc. almost any type of perfume. Its sweetness, versatility and very low cost makes it almost universally applicable. For Rose, Jasmin, Hyacinth, Reseda, Freesia, Peony, Magnolia, Oriental and even citrusy fragrance types, it may be used at concentrations from 1 percent up to 10 or perhaps much higher.

The title ester is also commonly used in flavor compositions, for imitation Butter, Apple, Apricot, Caramel, Honey, Passionfruit, Peach, Strawberry and fruit complexes, Vanilla flavors, floral and Rose type flavors, etc.

The concentration in the finished product is normally as low as 1 to 6 ppm.

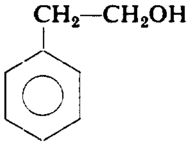
G.R.A.S. F.E.M.A. No.2857.

Prod.: by direct esterification of Phenylethylalcohol with Acetic acid or Acetic anhydride.

31-125; 33-502; 26-654; 61-71; 106-292; 140-136; 90-333; 156-311; 163-62; 163-232; B-VI-479;

## 2513: PHENYLETHYL ALCOHOL

Phenethylalcohol.
*beta*-Phenylethanol.
*1*$^{2}$-Oxy-*1*-ethylbenzol.
Benzyl carbinol.
*beta*-Hydroxy ethylbenzene.
*2*-Phenylethylalcohol.
Mellol (Bush-Boake-Allen).
Gallicol (Firmenich).
Phenarose (I.F. & F.).
Phenethylol.
P.E.A.



$C_8H_{10}O = 122.17$

Colorless oily liquid. Sp.Gr. 1.03.
B.P. 220° C.

2% soluble in water, except for commercial grade which may be only 1.5% soluble. Soluble in Propylene glycol, miscible with alcohol and oils.

Mild and warm, Rose-honey-like odor of moderate to poor tenacity. Poorer grades show earthy or pungent, more Hyacinth-like topnotes, or greener "gassy" notes. Very sensitive evaluation can be undertaken by smelling the aqueous solution. Most impurities are insoluble in water and will show up many times stronger, while the pure alcohol only smells mild, rosy in water.

Water is soluble in Phenylethylalcohol at the rate of 9%.

The alcohol has a measurable bactericidal effect at concentrations higher than 0.5% (in water).

The taste of this alcohol is sweet and Honey-rose-like at concentrations lower than 40 ppm, but tends to become unpleasantly perfumey at higher concentrations.

Phenylethylalcohol is one of the most widely used of all perfume chemicals. The annual production in the United States of America is now over 2 Million pounds, although only one manufacturer is making the alcohol on a continuous scale.

This material enters perfume compositions at the rate of 5-10-20% or sometimes much more. Its low cost, versatility and general acceptability on odor, its excellent stability are factors speaking strongly in favor of this otherwise relatively weak odorant. However, its odor is clearly demonstrated in an experiment with an apparently weak crystalline fixative/odorant, such as Trichloro methyl phenyl carbinyl acetate (Trirosol, Rosetone, etc.). With 5% of the crystalline material, Phenylethylalcohol will smell not only much more rosy, it will last much longer, and its "rough" topnotes are pleasantly subdued, it has "three dimensions" instead of two.

But it is in the "everyday" perfumery that the subject alcohol is most appreciated. It is almost never "out of place" in a composition, be it floral, balsamic, Oriental, mossy, herbaceous or "modern-aldehydic". It is an inevitable companion to the "rose alcohols", Citronellol, Geraniol, Nerol, Dimethyloctanol, etc. and it may receive fixation from Guaiacwood oil, Nitromusks, Coumarin and Heliotropine, Rosetone, Resinoids, etc. It blends excellently with the Linalool family, and with all the newer "Lily"-alcohols, "Muguet"-alcohols, etc. as well as in Lime and Spice blends.

The title alcohol finds some use in flavor compositions, mainly in imitation Butter, Strawberry, Raspberry (very common ingredient), Caramel, Honey, Melon, and in various fruit complexes, etc.

The concentration used is normally low, about 0.1 up to 20 ppm, but most often near 1-3 ppm.

G.R.A.S. F.E.M.A. No.2858.

Prod.:

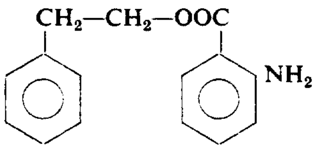
1) from Styrene oxide by hydration.
2) from Ethylene oxide and Benzene with Aluminium chloride.

Many other methods are in use, but method No. 1) may – with certain modifications – become the modern and future method for large-scale production.

26-654; 68-499; 100-792; 106-293; 140-130; 156-306; 160-1152; 163-62; 163-232; 163-371; B-VI-478;

## 2514: PHENYLETHYL ANTHRANILATE

*beta*-Phenethyl-*ortho*-aminobenzoate.
Benzylcarbinyl anthranilate.
"Graposynth".



$C_{15}H_{15}NO_2 = 241.29$

White crystalline mass, colorless crystals or straw-colored, fused mass (poorer grades, old process).

M.P. 42° C. B.P. 324° C. Sp.Gr. 1.14 (liquid).

Insoluble in water, soluble in alcohol and oils.

A very pure material is virtually odorless, but odor descriptions are almost exclusively based upon testing of old material, manufactured by an unsatisfactory process (see below).

In spite of the apparent absence of odor, the material has an unquestionable effect when incorporated in a composition along with more volatile, odorous chemicals.

Its effect is then sweet-floral, deep-fruity, herbaceous-honey-like and it has outstanding tenacity.

The ester is used in perfume compositions for its sweet-fruity floral effect in Gardenia, Honeysuckle, Violet, Plumeria (Frangipanni), etc. It blends very well with the Ionones and Methylionones for above purposes, and it should be kept in mind that this ester will form "Schiff's bases" with most aldehydes. Not all of these Shiff's bases are desirable – of color or odor.

The ester finds use in flavor compositions for its Grape- and Grapefruit-like effect, which is only obvious at very low concentrations. The taste is very perfumey at 20 ppm or higher, while near 1 ppm it becomes sweet and fruity, Grape-like, jam-like.

It is also used in Butter flavors, Caramel and Honey, and as a fixative in various fruit complexes. The concentration in the finished product will be about 1 to 6 ppm.

G.R.A.S. F.E.M.A. No.2859.

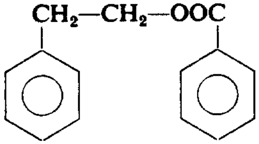
Prod.:

1) from Phenylethyl alcohol and Methylanthranilate. This produces a fairly pure ester, but it will contain perceptible amounts of Methylanthranilate.
2) Phenylethyl alcohol plus Isatoic anhydride produces a very high grade material, provided equipment is modern and vacuumdistillation perfected.

34-1012; 106-295; 163-62;

## 2515: PHENYLETHYL BENZOATE

Phenethyl benzoate.



$C_{15}H_{14}O_2 = 226.28$

Colorless oilyl liquid. Sp.Gr. 1.10.
B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Very faint floral-balsamic odor reminiscent of dry Rose leaves and petals with a soft, honey-like undertone and excellent tenacity.

The odor of this ester may not impress the observer on the first encounter, but in use it displays very attractive effects, other than the fixative effect.

The material is used in Carnation, Neroli, Rose and Oriental bases mostly as a fixative, but also as a blender/modifier in the heavier portion of the fragrance. It is a good base for Peony and other delicate florals, and it blends well with most of the conventional "middle notes".

This material is also used in flavor compositions in minute traces for fixation of Honey, Strawberry and various fruit types.

The concentration is normally as low as 1 to 4 ppm in the finished product.

Prod.:

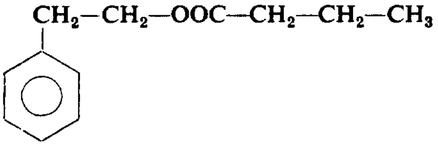
1) from Phenylethylalcohol and Methylbenzoate.
2) by azeotropic esterification of Phenylethylalcohol with Benzoic acid.

G.R.A.S. F.E.M.A. No.2860.

26-654; 106-296; 163-62;

## 2516: PHENYLETHYL BUTYRATE

*beta*-Phenethyl-*n*-butanoate.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Sp.Gr. 1.00. B.P. 238° C.

Practically insoluble in water, soluble in alcohol and oils.

Fine and natural-rosy, warm, floral-fruity odor of moderate tenacity. The material must be free from Butyric acid, and if it is properly cleaned, it keeps well under normal storage conditions. Yet, it is generally considered less stable than the *iso*-Butyrate (see next).

This ester finds use in perfumes of the Jasmin, Honey, Hyacinth, Magnolia, Freesia, Frangipanni, Ylang, Lily, Lilac and many other sweet-floral types. Traces are used in Tuberose, and the material may be used by some perfumers for part of an "animal-floral" effect. This could, however, be ideas carried over from the time when the ester was brought on the market in an unsatisfactory grade.

The title ester is used in flavor compositions for imitation Strawberry, Butter, Caramel, Apple, Peach, Pineapple, Tobacco flavors, Honey bases, Floral bases, etc. in concentrations equal to 3 to 15 ppm in the finished consumer product.

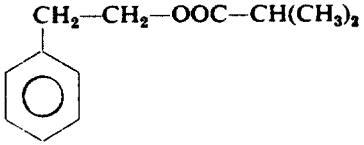
G.R.A.S. F.E.M.A. No.2861.

Prod.: by direct esterification of Phenylethyl alcohol with *n*-Butyric acid, e. g. under azeotropic conditions.

33-732; 61-71; 106-297; 156-311; 163-232; 163-62;

## 2517: PHENYLETHYL-iso-BUTYRATE

*beta*-Phenethyl-*iso*-butyrate.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Sp.Gr. 1.00. B.P. 230° C.

Insoluble in water, soluble in alcohol and oils.

Refreshing fruity-rosy odor. More fruity than rosy, and overall fresher than the *n*-Butyrate. Moderate to poor tenacity.

Pleasant fresh-fruity, Strawberry-Pineapple-like taste in concentrations below 20 ppm. Taste is vastly improved in presence of mild food acid.

This ester finds as much use in perfumery as does the *n*-Butyrate. There seems to be two schools of opinions, one who prefer the *n*-Butyrate, and another preferring the *iso*-Butyrate. Few perfumers use both, although one should think it would be a healthy idea for elimination of psychological antipathy or subconscious reluctance in using certain materials, if the immediate odor impression has not been favorable. But the human element of subconscious reaction is very difficult to eliminate, and it affects the creative perfumer as well as any other person.

The title ester is used for Jasmin, Hyacinth, Rose, Peony and many other fruity-floral types, also in Gardenia, Honeysuckle, Frangipanni, etc.

In flavors, it finds use for imitation Apple, Peach, Pineapple, Strawberry, Honey, Cheese, and in various floral and fruity complexes.

The concentration is relatively low, about 5 to 15 ppm in the finished product.

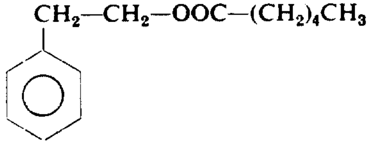
G.R.A.S. F.E.M.A. No.2862.

Prod.: by direct esterification of Phenylethylalcohol with *iso*-Butyric acid, e. g. under azeotropic conditions.

33-732; 140-140; 106-300; 163-62; 163-233;

## 2518: PHENYLETHYL CAPROATE

*beta*-Phenethyl hexoate.
Phenylethyl hexanoate.
Benzyl carbinyl hexylate.



$C_{14}H_{20}O_2 = 220.31$

Colorless oily liquid. Sp.Gr. 0.98.
B.P. 263° C.

Practically insoluble in water, soluble in alcohol and oils.

Fruity-green, rosy, fresh-Pineapple-like, Banana-like odor type of good tenacity.

In concentrations below 10 ppm, the taste is pleasant, resembling that of unripe Pineapple-Banana, yet sweet and fresh. Higher concentrations seem to emphasize the green-metallic notes in the ester.

This ester may be used in perfumery, but the author believes that its use as such is very rare.

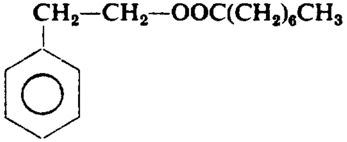
It is used in flavor compositions as modifier in Banana, Pineapple, Strawberry, Peach and other imitation flavors. The concentration is usually about 2 to 8 ppm in the finished product, but the title ester is not included in the American G.R.A.S. list and it can therefore not be used in food flavors in the U.S.A.

Prod.: by direct esterification of Phenylethylalcohol with *n*-Hexanoic acid under azeotropic conditions.

34-1230; 163-232;

## 2519: PHENYLETHYL CAPRYLATE

Phenethyl octoate.
Phenylethyl octanoate.
Benzyl carbinyl octylate.



$C_{16}H_{24}O_2 = 248.37$

Colorless oily liquid. Sp.Gr. 0.95.
B.P. 295° C.

Insoluble in water, soluble in alcohol and oils.

Mild, fruity-winey odor with a peculiar herbaceous-earthy, almost fungoid character, not uncommon in C-8 derivatives.

Mild, fruity-winey taste in concentrations below 10 ppm, but rather perfumey-bitter at higher levels.

This ester is rarely offered commercially. It is occasionally used as a modifier in Oriental-Rose type fragrances, where it performs very well with Patchouli and Opopanax. It is also interesting in Lavender and Clary Sage, as its tenacity is quite good.

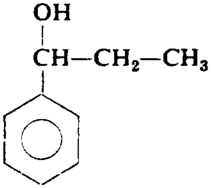
The author has no record of its use in flavors.

Prod.: by azeotropic esterification of Phenylethyl alcohol with *n*-Octanoic acid.

156-311; 163-232;

## 2520: PHENYL ETHYL CARBINOL

*1*-Phenyl-*1*-propanol.
Ethyl phenyl carbinol.
*secondary*-Phenyl propyl alcohol.
"Dihydro-*iso*-cinnamic alcohol".
Dihydro-*alpha*-phenyl allyl alcohol.



$C_9H_{12}O = 136.20$

Colorless oily liquid. Sp.Gr. 0.99.
B.P. 220° C.

Insoluble in water, soluble in alcohol and oils.

Pleasant floral-balsamic odor, somewhat more powerful than Phenylpropyl alcohol, and not as "delicate". Moderate to poor tenacity.

Sweet balsamic-honey-like taste in concentrations below 5 ppm, but higher concentrations appear "perfumey".

The title alcohol is very rarely used in perfumes, but could find some application as a modifier for Phenylpropylalcohol in Hyacinth, Rose, Lilac, Magnolia, etc.

The material finds some use in flavor compositions, almost exclusively in imitation Honey and in various fruit complexes. The concentration used is normally as low as 0.5 to 2 ppm in the finished product.

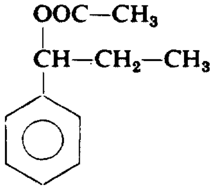
G.R.A.S. F.E.M.A. No.2884.

Prod.: by hydrogenation of Phenylethyl ketone (= Propiophenone).

26-548; 163-371; B-VI-502;
see also: Phenyl allyl alcohol.

## 2521: PHENYLETHYL CARBINYL ACETATE

Ethyl phenyl carbinyl acetate.
*secondary*-Phenyl propyl acetate.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Fresh-floral and fruity-balsamic odor of moderate tenacity. The floral notes are mildly rosy, the fruity are reminiscent of Raspberry, but the odor is overall very mild and quite versatile, although it carries a touch of greenness.

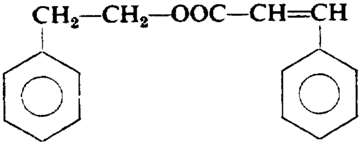
However, it seems that this ester is very rarely used in perfumery, at least under its proper chemical name. It may form part of various successful specialties, but the material is not often offered commercially.

It blends well with Ylang, Methylionones, Citronellol, Geraniol, Linalool, Hydroxycitronnellal, etc. and it can be used at relatively high level. As a distinctly floral material, however, it does not match the much more popular Dimethyl benzyl carbinyl acetate.

Prod.: by direct esterification of Phenylethyl carbinol with Acetic acid under azeotropic conditions.

## 2522: PHENYLETHYL CINNAMATE

Phenethyl cinnamate.
Benzyl carbinyl cinnamate.
*beta*-Phenylethyl-*3*-phenylpropenoate.



$C_{17}H_{16}O_2 = 252.32$

White crystals or amorphous powder.
M.P. 58° C. (The melting point varies considerably in products of different origin).
B.P. over 300° C.

Insoluble in water, slightly soluble in cold alcohol, soluble in hot alcohol and oils.

Very faint, but sweet and pleasant, balsamic odor of excellent tenacity. There is a mild, floral-fruity note in the sweetness of a very pure material.

In very low concentrations, this fruity note is more clearly detected as a fruity-sweet, Plum-like taste – at about 5 ppm or lower.

This ester is used quite frequently in perfume compositions in spite of its poor solubility, which is hardly a problem at concentrations below 5%. As a background note and part of a fixative base, this material finds its way into Muguet, Rose, Lilac, Sweet Pea, Gardenia, Magnolia, Peony, Hyacinth and many types of Oriental fragrance. Its effect could be classified as "Tolu-balsam-like", although it does not carry the intense sweetness and complexity of the natural balsam. It is particularly good in the very mild and delicate florals.

In flavors, traces are used for fixation of fruity-jam-like notes, e. g. in Plum, Prune, Cherry and various fruit complexes.

The concentration will be about 0.1 to 3 ppm in the finished product.

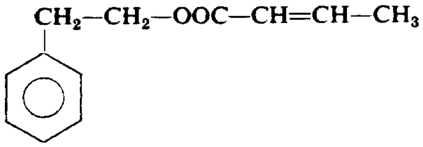
G.R.A.S. F.E.M.A. No.2863.

Prod.: (several methods) e. g. from Phenylethylalcohol and Methylcinnamate by "alcohol interchange esterification".

26-654; 34-462; 90-348; 163-62; 106-298; 163-232;

## 2523: PHENYLETHYL CROTONATE

Phenethyl-*trans-2*-butenoate.



$C_{12}H_{14}O_2 = 190.24$

Colorless oily liquid. Sp.Gr. 1.02.
B.P. 271° C.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant, dry-and-sweet, mildly rosy-musty odor with warm-herbaceous undertone. Tenacity is good.

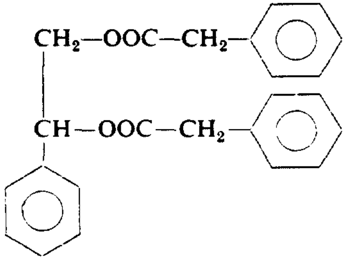
This ester is used in perfume compositions for floral, Oriental, balsamic and herbaceous fragrance types, mainly as a modifier, a warm undertone and as a supporting note to Labdanum, Rose, Sandalwood, Opopanax, Methylionones, Lavender and many other fragrance materials. It works particularly well with Opopanax.

Prod.: from Phenylethyl alcohol and Crotonic acid by azeotropic esterification.

(Sample: Norda Ess. Oil & Chem. Co.).

## 2524: PHENYLETHYLENEGLYCOL DIPHENYLACETATE

Phenyl-*1,2*-ethanediol di-phenylacetate.



$C_{24}H_{22}O_4 = 374.44$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Extremely tenacious, warm and mild-rosy, earthy-honey-like odor.

This ester, known for a very long time under trade name of a German chemical company, is still used in perfume compositions and bases. It was also incorporated in various successful specialties.

There is considerable difference in the odor of materials manufactured by different companies, and there is also a difference of opinion as to how the material "should smell". A small surplus of Phenylacetic acid will dominate the odor, while some perfumers actually prefer at least a trace of that odor. The very pure (chemically balanced) ester has only a very faint odor, but it still has considerable effect in a perfume composition, most perceptible in presence of more volatile components.

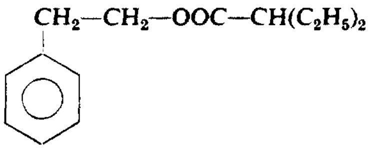
This material is used mainly for rose variations, as a modifier in Oriental-sweet types, l"Origan"-types, etc. or in new versions of Chypre. It is also very pleasant as a background in Reseda-notes.

Prod.: by esterification of Phenylethylene glycol with Phenylacetic acid in presence of a catalyst, e. g. Aluminum phosphide.

(Agfa-sample).
See also 2574 (Monoacetate).

## 2525: PHENYLETHYL-2-ETHYLBUTYRATE

Phenethyl diethylacetate.
Diethylacetic acid, Phenylethylester.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Delicate, fresh-fruity-rosy odor of considerable tenacity.

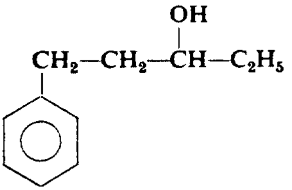
This rare ester is used in perfumery, although not often offered commercially under its proper chemical name. It finds its way mainly into specialties and bases, manufactured by the user himself, and therefore not found on the perfumer's shelf.

It introduces very natural rosy notes and fruity-herbaceous undertones when used at 2-4% in a Rose base. For novel effects it can be used at much higher level of concentration since it does not tend to dominate a fragrance. It blends very well with Dimethyl octanol and its esters, with Phenylethyl propionate, etc.

Prod.: by direct esterification of Phenylethyl alcohol with Diethylacetic acid under azeotropic conditions.

## 2526: PHENYLETHYL ETHYLCARBINOL

*5*-Phenylpentan-*3*-ol.
Ethyl phenylethyl carbinol.



$C_{11}H_{16}O = 164.25$

Colorless liquid, solidifying in the cold.
B.P. 224° C. Sp.Gr. 1.01.

Almost insoluble in water, soluble in alcohol and oils.

Warm-balsamic, floral and slightly earthy-green-spicy odor of moderate tenacity.

This carbinol finds a little use in perfumery, although it is far from being a common ingredient.

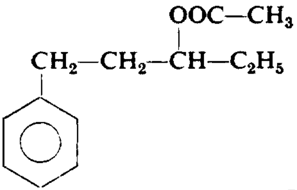
For carnation, Ylang-Ylang, Wallflower, etc. it may be used as a modifier or supporting note, a blender to the more spicy materials, a liaison between the floral and the spicy notes.

Prod.:
1) by hydrogenation of Phenylethyl ethyl ketone.
2) from Phenyl propionic aldehyde and Ethyl magnesium bromide in a Grignard type reaction.

163-62;

## 2527: PHENYLETHYL ETHYL CARBINYL ACETATE

*5*-Phenylpentan-*3*-yl acetate.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid. B.P. 228° C.
Sp.Gr. 1.00.

Practically insoluble in water, soluble in alcohol and oils.

Fresh-floral, mildly green-rosy and discretely balsamic odor of moderate tenacity. Overall more "lively" than the carbinol (see previous).

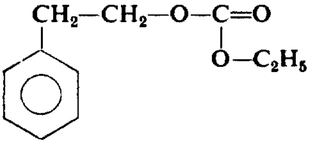
Although the odor and type of this ester are actually very pleasant and useful, the material is not a common one, and it is rarely offered under its proper chemical name.

In competition with the many excellent and more versatile carbinols and esters, this material will probably not be able to survive, and it is reasonable to predict that it is about to become obsolete.

Prod.: by azeotropic esterification of Phenylethyl ethylcarbinol with Acetic acid.

163-62;

## 2528: PHENYLETHYL ETHYLCARBONATE



$C_{11}H_{14}O_3 = 194.23$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Pleasant ethereal-alcohol-like, sweet and rather powerful odor of poor tenacity.

The title material finds some use in perfume compositions as part of topnote compositions, floral bases and certain types of herbaceous fragrance. It blends well with Lavender and Clary Sage, and it has a mellowing effect upon the alifatic aldehydes in aldehydic top-note bases, etc.

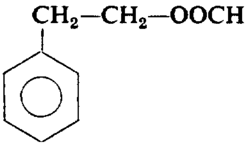
The ester is also interesting by its effect of "lifting" a musk odor so that the musk becomes perceptible at a much earlier stage of the perfume evaporation. In a way, the opposite of a fixative effect, but quite attractive when used with the proper amount and type of musk.

Prod.: from Ethyl monochloroformate and Phenylethylalcohol in Chloroform with Pyridine as a catalyst.

31-138;

## 2529: PHENYLETHYL FORMATE

Phenethyl methanoate.
Benzyl carbinyl formate.



$C_9H_{10}O_2 = 150.18$

Colorless liquid. Sp.Gr. 1.03. B.P. 226° C.

Powerful, green-herbaceous, rosy odor with some similarity to Chrysanthemum, Hyacinth and Watercress foliage. Moderate to poor tenacity.

This ester is suprisingly rare in perfume formulations, although it probably is available in almost any perfume laboratory. One reason for its infrequent use may be that it does not keep well if it has not been prepared in the proper quality in the first place. If traces of water or formic acid were present from the beginning, the material will not only show pungent and unpleasant odor, but it will deteriorate rapidly and increase further in acidity.

However, a properly made ester, kept dry and cool, will keep excellently on the perfumer's shelf, and its odor remains warm, green-herbaceous and floral.

The ester is an excellent modifier in Muguet, Orchid, Lilac, Rose, Narcisse, and, in larger amounts, in Hyacinth. It is interesting to note once more the enormous difference between the Formates and the Acetates while there is not nearly the same type-difference between the Acetates and the Propionates, etc.

Generally, formates are neglected in perfumery, perhaps partly because of above mentioned problem. But their warm, dry-foliage type floral odor lends very natural and attractive effects to a fragrance.

The title ester is also used in flavor compositions, mainly in berry complexes, and in Apple, Apricot, Banana, Cherry, Honey, Peach, Pear, Plum, etc.

Concentration in the finished product is about 1 to 15 ppm.

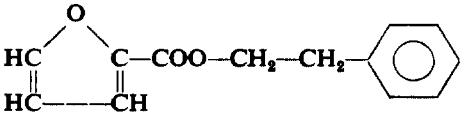
G.R.A.S. F.E.M.A. No.2864.

Prod.: by cold formylation of Phenylethyl alcohol.

31-134; 106-299; 163-63; 163-232; 140-133;

## 2530: PHENYLETHYL-2-FUROATE

Phenethyl furoate.
Benzyl carbinyl-*alpha*-furan carboxylate.



$C_{13}H_{12}O_3 = 216.24$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Warm, fruity-caramellic, slightly earthy-oily odor of moderate tenacity.

Warm, oily-caramellic, slightly but pleasantly fungoid taste in concentrations below 2 ppm.

The title ester is not used in perfume compositions as far as the author is aware.

It is used in trace amounts in flavor compositions for its peculiar warm notes, mainly in Chocolate and Mushroom imitation flavors.

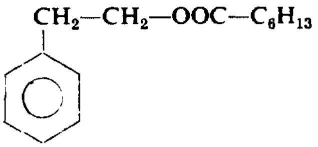
The concentration in the finished product may be as low as 0.05 ppm.

Prod.: by azeotropic esterification of Phenylethylalcohol with Furan-*2*-carboxylic acid.

G.R.A.S. F.E.M.A. No.2865.

## 2531: PHENYLETHYL HEPTOATE

Phenethyl heptanoate.
Phenylethyl heptylate.
Benzyl carbinyl heptoate.



$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. Sp.Gr. 1.01. B.P. 273° C.

Insoluble in water, soluble in alcohol and oils.

Mild, oily-citrusy-fruity odor of Orange character but with distinctly earthy-herbaceous notes, almost fungoid. Good tenacity.

This ester is occasionally used in perfume compositions, where it can blend very attractively in Lavender and Bergamot, while in floral fragrance types, it has a mellowing effect.

It is rarely offered commercially, but usually prepared by the interested party for "captive" use in own formulations.

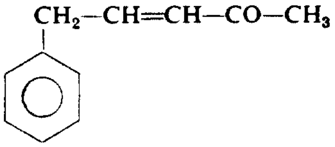
However, its effect is apparently not sufficiently unusual that it can become a common market item.

Prod.: by azeotropic esterification of Phenylethyl alcohol with Heptanoic acid.

35-61; 163-63; 163-232;

## 2532: PHENYLETHYLIDENE ACETONE

*5*-Phenyl-*3*-penten-*2*-one.



$C_{11}H_{12}O = 160.22$

Colorless to pale yellowish oily liquid, solidifying in the cold.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, floral-green, sweet and tenacious odor.

This ketone, curiously enough, is very rarely offered commercially under its proper name. It has been used in several well known specialties, mostly of the sweet-floral type.

The title material lends power and intense sweetness, combined with discretely green notes to a composition, and is therefore suitable for Sweet Pea, Honeysuckle, etc. The material must be used with discretion, however, since it is relatively powerful and penetrating.

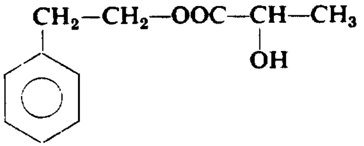
Being a higher homologue of Benzylidene acetone, the title material is exposed to much of the same suspicion and reluctance in use as that material – assuming that this type of ketone may be a hazard to human skin. Published reports have not yet confirmed this about the title material, and the normal, discrete use-level should present no such hazard.

Prod.: by condensation of Phenylacetaldehyde with Acetone.

7-243; 7-340; 7-385; 31-84; 61-67;

# 2533: PHENYLETHYL LACTATE

Phenethyl-2-hydroxypropanoate.
Benzyl carbinyl-*alpha*-hydroxypropionate.



$C_{11}H_{14}O_3$ = 194.23

Colorless, slightly viscous liquid.

Slightly soluble in water, miscible with alcohol and oils.

Very faint, bland-sweet, fruity-ethereal odor, sometimes with a rosy note, presumably derived from a surplus of the alcohol parent.

This ester is briefly mentioned because it has occasionally been used as a "blender" or little more than a solvent/diluent in perfume compositions, and in Raspberry flavor compositions.

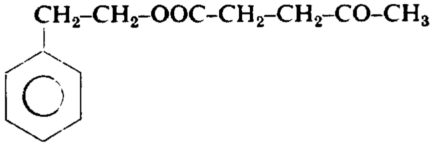
It is normally not considered a fragrance material, and it has no importance in perfumery.

The use in flavor creation is also very rare. The effect is weak and uninteresting, but the material does have some mellowing effect upon certain types of fruit flavor imitation.

Prod.: by azeotropic esterification of Phenylethyl alcohol with Lactic acid.

# 2534: PHENYLETHYL LEVULINATE

Phenethyl laevulate.
Phenylethyl-*gamma*-keto-valerate.



$C_{13}H_{16}O_3$ = 220.27

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm, ethereal-herbaceous, also caramellic-sweet odor of moderate tenacity.

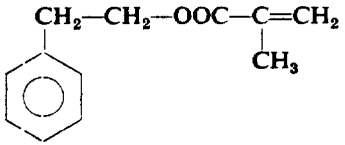
The title ester is used in perfume formulations to a minor degree, but it is rarely offered commercially. It is also used as part of various specialties, known under trade names.

It is a type of fragrance chemical with rather versatile uses: It will enhance Labdanum in sweetness and winey topnotes, while it will add life to an overly "chemical" rose composition. It is not confined to these types, but can be applied to almost any type of floral and sweet-herbaceous fragrance, including Lavender, Oriental, Fougère, fruity and Tobacco-like types.

Prod.: by azeotropic esterification of Phenylethylalcohol with Levulinic (Laevulic) acid.

# 2535: PHENYLETHYL METHACRYLATE

Phenethyl-2-methylpropenoate.
Benzyl carbinyl-*alpha*-methylacrylate.



$C_{12}H_{14}O_2$ = 190.24

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Dry-and-sweet, ethereal-herbaceous rose odor of moderate to poor tenacity. The rosy notes are more "dry-leaf"-notes than truly floral notes, a fact which gives impression of "Potpourri-rose", or the old-fashioned Rose-sachets.

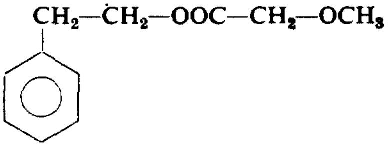
This ester finds use in perfume compositions, including soap perfumes where it may lend warmth and pleasant "dried-leaf" notes to a Rose or an Oriental type fragrance. It blends well with the Methylionones, Cedarwood products, Jasmin materials, Sandalwood notes, etc. and it can be used in relatively large amounts.

There are very few manufacturers of this chemical, but it is available under its proper name. Yet, it is not commonly found on the perfumer's shelf.

Prod.: by azeotropic esterification of Phenylethylalcohol with 2-Methylpropenoic acid.

163-233;

## 2536: PHENYLETHYL METHOXYACETATE



$C_{11}H_{14}O_3 = 194.23$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Fresh and sweet, rosy-fruity odor of moderate to poor tenacity. More rosy than fruity, and not quite as sweet as Phenylethyl acetate.

This ester has been suggested for use in perfume compositions, but it is possible that it is only very rarely used, or not used at all. It does not display any particularly attractive notes or effects which can not be obtained from the conventional materials.

It is briefly mentioned here as an example of this particular ester series which, incidentally, does not produce many materials of perfumery interest.

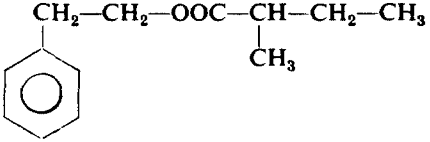
The title material has a slightly burning taste in concentrations near 20 ppm, and it is bitter even below that level. It is therefore unlikely that the material can find use in flavors.

Prod.: by direct esterification of Phenylethylalcohol with Methoxyacetic acid.

31-159;

## 2537: PHENYLETHYL-2-METHYLBUTYRATE

Phenethyl-*alpha*-methylbutanoate.
Benzyl carbinyl ethyl methyl acetate.
*active*-Valeric acid, Phenylethyl ester.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, floral-fruity odor with a warm, oily-herbaceous undertone and moderate tenacity.

Sweet and mildly fruity, oily herbaceous taste in concentrations below 10 ppm. The taste is pleasant at considerably higher level.

This ester has found some use in flavor compositions, mainly in imitation Peppermint, which is still a very difficult problem in spite of intense and very fruitful research into that oil.

The author is not aware of any use of this ester in perfume compositions.

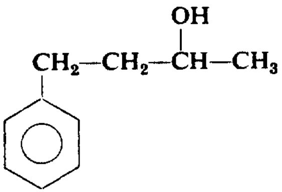
G.R.A.S. (cleared for use in food flavorings, by the Federal Register).

Prod.: by azeotropic esterification of Phenylethyl alcohol with *alpha*-Methylbutyric acid.

NOTE: A number of esters of this acid have been identified in natural essential oils, and most of them have subsequently been included in the American G.R.A.S. list as permitted for use in food flavors.

## 2538: PHENYLETHYL METHYL CARBINOL

*dl-4*-Phenyl-*2*-butanol.



$C_{10}H_{14}O = 150.22$

Colorless liquid. B.P. 229° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and warm, herbaceous-fruity odor of moderate tenacity.

The taste is rather sweet in concentrations below 20 ppm, but the fruity note is nondescript, yet warm and pleasant. Higher concentrations are less pleasant, more "chemical".

This "carbinol" finds use in flavor compositions as a modifier in fruit complexes, etc. where it can blend the more chemical and volatile materials into an attractive and harmonious composition. The carbinol will supply the greener portion of the fruity notes, yet it will also lend some sweetness.

The concentration used is about 0.5 to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2879.

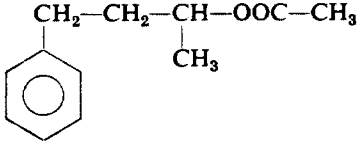
Prod.:

1) by hydrogenation of Benzylacetone.
2) from Phenylpropionic aldehyde and Methyl magnesium bromide in a Grignard type reaction.

68-501;

## 2539: PHENYLETHYL METHYL CARBINYL ACETATE

*4*-Phenyl-*2*-butanol acetate.
(Not to be confused with Butyl phenylacetate).



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild and fresh, slightly green, fruity and sweet odor of moderate tenacity.

Sweet fresh-fruity, mild taste with a green, peel-like note in concentrations below 10 ppm.

The title ester is, to the author's knowledge, not used commonly in perfumes.

It finds some use in flavor compositions of the Peach, Apricot and Mango type, where it blends excellently with Undecalactone and alkyl caproates, etc.

The normal concentration in finished products will be as low as 0.2 to 5 ppm.

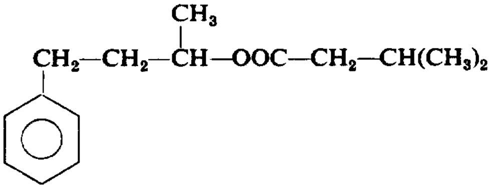
G.R.A.S. F.E.M.A. No.2882.

Prod.: by azeotropic esterification of Phenylethyl methyl carbinol with Acetic acid.

61-71;

## 2540: PHENYLETHYL METHYL CARBINYL-iso-VALERATE

*4*-Phenyl-*2*-butanol-*iso*-valerate.



$C_{15}H_{22}O_2 = 234.34$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild, but tenacious, sweet, green-fruity, warm-herbaceous odor.

Sweet, mildly green herbaceous-fruity, very pleasant taste in concentrations near 5 ppm.

This ester, very rarely offered commercially under its proper chemical name, is used in flavor compositions as a modifier and blender in Apple, Tobacco, Strawberry, Plum and many other fruit types, but always at very low concentration, about 1 ppm in the finished product, often much lower.

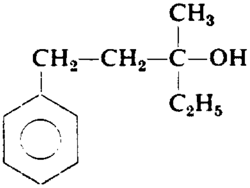
Its fixative power makes it particularly suitable for blending into compositions of volatile esters, and its herbaceous, fresh-tobacco-like character offers good effects in Tobacco flavor compositions.

The author has no report of its use in perfume compositions, but it could undoubtedly find use in Fougères, Chypres, Oriental fragrance types, etc. as a modifier, and in topnote compositions as a novel type fixative for green-fruity topnotes.

Prod.: by azeotropic esterification of Phenylethyl methyl carbinol with *iso*-Valeric acid.

## 2541: PHENYLETHYL METHYL ETHYL CARBINOL

*1*-Phenyl-*3*-methyl-*3*-pentanol.
*3*-Methyl-*1*-phenyl-*3*-pentanol.
Methyl ethyl phenylethyl carbinol.
P.E.M.E.C.



$C_{12}H_{18}O = 178.28$

Colorless, slightly viscous liquid.
B.P. 254° C. Sp.Gr. 0.97.

Almost insoluble in water, soluble in alcohol and oils.

Mild, warm-rosy and floral, refreshingly Muguet-like and tenacious odor. Delicate, fruity-green taste in concentrations below 5 ppm.

This higher homologue of one of the most exquisite of all the carbinols (Dimethyl phenylethyl carbinol) is used in perfume compositions, but on account of its relatively high cost, it is more or less reserved for finer cosmetic fragrances and handkerchief(lotion) perfumes, etc.

The title carbinol is almost born to be a rose base material. Its warmth and refined powdery-sweet note with a delicate touch of greenness makes it immediately attractive and tempting to use in Rose, Muguet, Lilac (it has the refined warmth of natural Cinnamic alcohol from Styrax) as well as Carnation, Chypres, etc.

Unfortunately, it is missing from many perfume laboratories, and therefore also from the minds of too many perfumes. From a chemical point of view, an increased interest and volume use of this material could undoubtedly bring its price down to a very attractive level and subsequently further increased use.

Its low vapor pressure may tempt the observer to think that it is a weak odor, but it is certainly not. Its power is also demonstrated in flavors, where traces of about 1 ppm are quite perceptible with warm-fruity notes. Its fixative effect is also utilized in various fruit complexes, and the concentration in finished products is normally as low as 0.2 to 0.8 ppm.

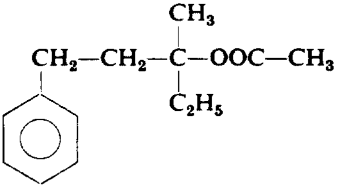
G.R.A.S. F.E.M.A. No.2883.

Prod.: from Phenylethyl magnesium bromide plus Methyl ethyl ketone in a Grignard type reaction.

34-162; 103-291; 156-76; 163-63; 163-233;

## 2542: PHENYLETHYL METHYL ETHYL CARBINYL ACETATE

Methyl ethyl phenylethyl carbinyl acetate.
*1*-Phenyl-*3*-methyl-*3*-pentanol, acetate.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid. Sp.Gr. 0.95. B.P. 262° C.

Practically insoluble in water, soluble in alcohol and oils.

Fresh, green-floral, Narcissus-Hyacinth-Lily type odor of good tenacity.

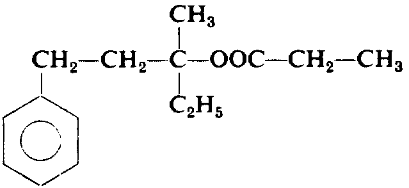
This ester is used to a limited extent in perfumery, but it does not seem to have achieved the same popularity as its parent carbinol. It is much less rosy, and more suitable for Hyacinth (which is much less in demand as a fragrance type), yet it is fresher and livelier overall. It blends very well with the conventional Hyacinth materials, but it is necessary to reduce or omit the more pungent items from a Hyacinth if the title material is to be used. It would be wasted if any significant amount of Phenylacetaldehyde or Hydratropic aldehyde were present.

Prod.: by azeotropic esterification of the carbinol (see previous monograph) with Acetic acid.

34-162; 103-292; 156-76;

## 2543: PHENYLETHYL METHYL ETHYL CARBINYL PROPIONATE

*1*-Phenyl-*3*-methyl-*3*-pentanol, propionate.
Methyl ethyl phenylethyl carbinyl propanoate.



$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. Sp.Gr. 0.98. B.P. 267° C.

Insoluble in water, soluble in alcohol and oils.

Sweet, earthy-rosy, mildly fungoid or mushroom-like, but overall pleasant and warm odor of good tenacity.

This ester, although rarely offered commercially, is occasionally used in perfume compositions as a modifier in Rose, Hyacinth, Lilac and other florals as well as in Lavender and Chypre types, where a few percent may lend a very pleasant undertone and blend the herbaceous with the floral notes.

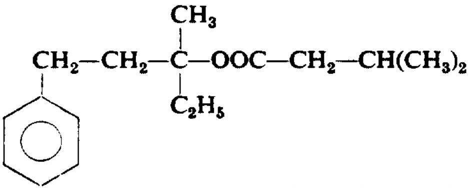
With the large variety of carbinols and esters on hand, this particular ester may not stand out as one of the indispensable ones, and most perfume laboratories may never have it on their shelf.

Prod.: by azeotropic esterification of Phenylethyl methyl ethyl carbinol with Propionic acid.

34-162; 156-76;

## 2544: PHENYLETHYL METHYL ETHYL CARBINYL-iso-VALERATE

*1*-Phenyl-*3*-methyl-*3*-pentanol, *iso*-valerate.
Methyl ethyl phenylethyl carbinyl-*iso*-pentanoate.



$C_{17}H_{26}O_2 = 262.40$

Colorless liquid. Sp.Gr. 0.97. B.P. 270° C.

Insoluble in water, soluble in alcohol and oils.

Mild and tenacious, herbal-fruity, warm odor with sweet-earthy notes.

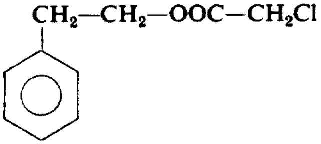
This ester is occasionally used in perfumery, although it is very rarely offered commercially. Its excellent tenacity and versatile odor characteristics makes it quite interesting for Chypre and modern creations as a liaison between the floral and the warm-herbaceous or woody theme. It works particularly well with Clary Sage absolute for such purposes.

Prod.: by azeotropic esterification of Phenylethyl methyl ethyl carbinol with *iso*-Valeric acid.

163-233;

## 2545: PHENYLETHYL MONOCHLOROACETATE

Phenethyl chloracetate.



$C_{10}H_{11}ClO_2 = 198.66$

Colorless oily liquid. Sp.Gr. 1.18.

Practically insoluble in water, soluble in alcohol and oils.

Faint and mild, but very tenacious, delicately rosy-honey-like odor. Undertones are discretely fruity, the floral notes resemble Freesia.

This ester is briefly mentioned as an example of the very few chlorinated perfume chemicals. Benzyl monochloroacetate is known, but the title material is very rarely found in a perfume laboratory. Part of the reason may be found in the psychological reluctance on the part of the perfumer against the use of any material bearing a name including "chloro-".

A well-balanced, correctly produced ester should, however, present absolutely no hazard of producing free Chlorine under normal perfume compound conditions.

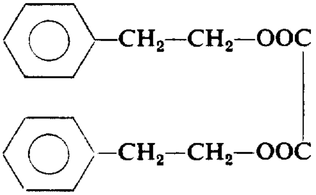
The ester could find use as a modifier in Rose, as a base in Peony and Freesia, a component of Carnation, Frangipanni, Magnolia, etc.

Prod.: by direct esterification of Phenylethyl alcohol with Monochloroacetic acid, e. g. under azeotropic conditions, but not necessarily so.

(Private experiments).

## 2546: PHENYLETHYL OXALATE

Diphenylethyl ethanedioate.



$C_{18}H_{18}O_4 = 298.34$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Weak and faint, oily-ethereal, sweet odor of good tenacity.

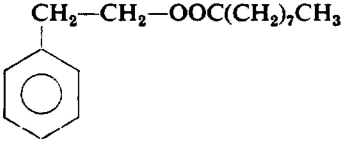
This ester has very little interest to perfumery, but it has been suggested as a fixative and solvent for mild floral fragrances, including Rose, Rose-Lavender, Lilac, etc. Its odor contribution is extremely small, and the material is actually dispensable since many materials of similar or better effects are available to the perfumer.

Prod.: by azeotropic esterification of Phenylethyl alcohol with Oxalic acid.

163-63;

## 2547: PHENYLETHYL PELARGONATE

Phenethyl nonanoate.
Benzyl carbinyl nonylate.



$C_{17}H_{26}O_2 = 262.40$

Colorless oily liquid. Sp.Gr. 0.95.
B.P. over 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Oily-sweet, delicately rosy, petal-like and mildly waxy, herbaceous odor of good tenacity.

This ester finds a little use in perfume compositions as a modifier for Rose bases and floral-herbaceous complexes. It performs best when both Rose and herbal notes are present, e. g. Lavender or Clary Sage, in Chypre and Fougère, etc.

Its taste is pleasantly winey-ethereal, sweet and discretely fruity at concentrations below 5 ppm.

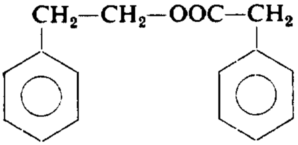
The ester is used in Wine and Cognac or Brandy flavor compositions but it is not included in the American G.R.A.S. list.

Prod.: by azeotropic esterification of Phenylethyl alcohol with Nonanoic acid.

163-63; 163-233; 163-371;

## 2548: PHENYLETHYL PHENYLACETATE

Phenethyl-*alpha*-toluate.
Benzyl carbinyl phenylacetate.
P.E.P.A.



$C_{16}H_{16}O_2 = 240.31$

Colorless crystalline mass. M.P. 28° C.
Sp.Gr. 1.09. B.P. 325° C.

The liquid material may remain supercooled as a viscous colorless liquid for a long time without forming crystals. Material of less than high chemical purity is usually liquid and does not crystallize.

Practically insoluble in water, soluble in alcohol and oils.

Heavy and very sweet, extremely tenacious, floral-balsamic odor which is sometimes described as "musky" (perhaps by observers who detect no special odor in the material), or "honey-like" (especially if it has surplus of Phenylacetic acid). A pure, well-balanced ester has only very faint Honey-character, and is mainly balsamic-rosy, intensely sweet, tenacious.

At concentrations of less than 10 ppm the taste is pleasantly sweet, Apricot-Nectar-like, but it is less pleasant, less natural at higher concentrations.

The title ester is one of the more popular Phenylethylesters. It is used at levels from about 1% up to more than 5% in a great variety of fragrance types other than Rose and Honey which are conventionally mentioned in connection with this material.

Its outstanding tenacity and good stability are utilized in soap perfumes where it may form part of the fixative base in floral, balsamic, Oriental and sweet-woody or tobacco-like types. It will support the musks and blend with Coumarin or the fruity lactone materials, improving the character of the fixative portion of a fragrance.

The ester is also used in fruit imitation flavor and Honey flavors. In Apricot it is quite a desirable item. The concentration in the functional consumer product will normally be about 2 to 10 ppm.

G.R.A.S. F.E.M.A. No.2866.

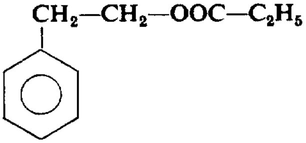
Prod.:

1) by azeotropic esterification of Phenylethylalcohol with Phenylacetic acid.
2) from Phenylacetyl chloride and Phenylethyl alcohol.

5-271; 34-246; 61-73; 56-209; 106-302; 163-63; 163-233;

## 2549: PHENYLETHYL PROPIONATE

Phenethyl propanoate.
Benzyl carbinyl propionate.



$C_{11}H_{14}O_2 = 178.23$

Colorless, slightly oily liquid. Sp.Gr. 1.02. B.P. 244° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Very warm, herbaceous-rosy, deep-fruity and moderately tenacious odor with a delicately spicy note (warm-balsamic).

Warm, sweet and herbaceous-deep-fruity taste of Strawberry-Raspberry type in concentrations near 20 ppm or lower. Tends to appear "perfumey" at higher levels.

This ester is, in the author's opinion, one of the most useful of all the derivatives of Phenylethyl alcohol. Its virtues are often vastly underestimated by many perfumers, and the material is left unused on the shelf in many laboratories.

Although it may not be the "key" ingredient, this ester is certainly supplying part of the most attractive and inimitable notes in many successful perfumes. Its floral supporting effect ranges from Ylang to Rose, from Jasmin to Lavender, and its warm, discretely spicy and balsamic effect can be utilized in almost any herbaceous, woody or Oriental type fragrance. It is a "classic" in "moss-rose", and it produces very rich and warm tonalities with the Benzoates, Salicylates, Styrax, Cinnamic alcohol, etc.

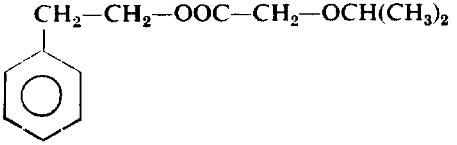
The title ester is used in flavor compositions for imitation Honey, Strawberry, Raspberry, Apricot, Peach, in fruit complexes and in tobacco flavorings. The concentration in the finished goods will be about 3 to 18 ppm.

Prod.: by azeotropic esterification of Phenylethyl alcohol with Propionic acid.

G.R.A.S. F.E.M.A. No.2867.

33-620; 103-107; 106-303; 163-63; 163-233;

## 2550: PHENYLETHYL-iso-PROPOXY ACETATE



$C_{13}H_{18}O_3 = 222.29$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Mild and refreshingly green, rosy odor of moderate to poor tenacity.

This ester has been suggested for use in perfume compositions, but it has no particular character or power, and it does not offer special effects which cannot be obtained from conventional materials. It has limited odor value, and mostly academic interest for the study of the odor of alkoxy acetates.

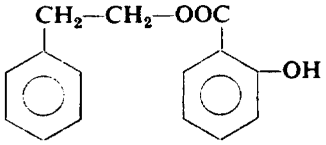
As compared to the lower esters (the -methoxy- is included in this work) it is greener and rosier, less fruity.

Prod.: by direct esterification.

31-159;

## 2551: PHENYLETHYL SALICYLATE

Phenethyl-*ortho*-hydroxybenzoate.
Benzyl carbinyl salicylate.



$C_{15}H_{14}O_3 = 242.27$

White granular crystals or crystalline powder. M.P. 44° C. B.P. over 300° C. Sp.Gr. 1.15 (liquid).

Practically insoluble in water, soluble in alcohol and oils.

Faint, but sweet and delicately balsamic-floral, Rose-Hyacinth and Carnation type odor of excellent tenacity.

At concentrations below 5 ppm the flavor is sweet, Apricot-like fruity or Honey-like, but at higher concentrations it is unpleasantly "chemical".

This material is very well known, but not extensively used. In competition with Benzylsalicylate which is liquid (a fact which psychologically appeals to perfumers) it is only a small item. And with the increasing talk about Benzylsalicylate being an offender in cosmetic preparations there could be even less use of this item.

Meanwhile, the ester enjoys much popularity from a group of steady users who know the virtues of this versatile material. As a fixative in Lily, Muguet, Lilac, Rose, Carnation, Honey, Clover, etc. it has excellent results on its record, and as a blender for highly "chemical" perfumes it can do small wonders. However, the title material does appear on the market in various grades, some of which are quite unacceptable, even some with phenolic off-odor. The ester blends particularly well with Cinnamic alcohol, Methylionones, Labdanum, the carbinols, etc. and as an undertone in more refined types of Fougère, it offers interesting possibilities.

The subject ester is used in flavor compositions, mainly imitation Peach, Apricot and Honey. The concentration is normally as low as 0.8 to 2 ppm in the finished product. Its mission is partly that of being a fixative, partly supplying the deep sweetness characteristic of those flavor types.

G.R.A.S. F.E.M.A. No. 2868.

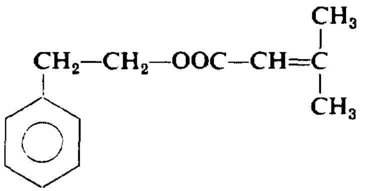
Prod.:

1) from Phenylethyl alcohol and Methyl salicylate by alcohol interchange reaction.
2) by azeotropic esterification of Phenylethyl alcohol with Salicylic acid.

34-788; 106-304; 163-63; 163-233;

## 2552: PHENYLETHYL SENECIOATE

Phenethyl-*3,3*-dimethyl acrylate.
Phenylethyl-*3*-methylcrotonate.



$C_{13}H_{16}O_2 = 204.27$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild, deep-sweet, herbaceous-winey, discretely floral-balsamic odor of moderate tenacity.

Sweet, ethereal-winey, deep-fruity taste in concentrations below 10 ppm. The fruity notes resemble Prune or other dried fruits.

This ester is very rarely offered commercially, and it is probably not used to any significant extent in perfumes.

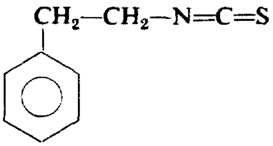
It finds use in flavor compositions as a modifier in various wine and Liqueur flavors, usually at concentrations equal to 5 ppm in the finished product. It acts partly as a fixative for the more volatile wine esters, partly as undertone of dried fruits, as a sweetener.

G.R.A.S. F.E.M.A. No.2869.

Prod.: by azeotropic esterification of Phenylethyl alcohol with *3*-Methylcrotonic acid.

## 2553: PHENYLETHYL-iso-THIOCYANATE

Phenethyl thiocarbimide.
Phenethyl mustard oil.
Resedalia.
Resedol.
Redol.
Resedozon.
Resedal.



$C_9H_9NS = 163.25$

Colorless to pale yellowish mobile liquid.
B.P. 256° C. Sp.Gr. 1.09.

Very slightly soluble in water, soluble in alcohol and oils.

Pungent, but rich and earthy-sweet, almost nut-like Radish-Horseradish-like odor, sometimes described as resembling the odor of crushed Rapeseed. The odor is considerably milder and less pungent than that of Benzyl-*iso*-thiocyanate.

This unusual material has achieved quite some fame as a "Reseda material par excellence" during many years while it was almost the only known chemical to smell like Reseda (underground parts). The odor of Reseda is not fashionable, and it does not seem to have "come-back's" such as for instance Lavender, Rondeletia, Oriental and other fragrance types.

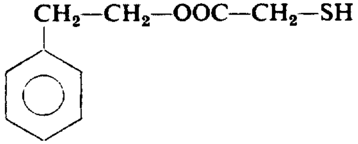
As a modifier in complex herbaceous-floral-woody fragrance types, the title material still finds some use, while the more sophisticated Acetals of Phenylacetaldehyde with various Glycols are being used as basis for Reseda fragrances or specialties.

Prod.:
1) from Phenylethyl amine with Carbon disulfide and basic Lead acetate.
2) or with Thiocarbonyl chloride.
3) or via the Sodium thiuramdisulfide plus Iodine to the title material.

7-340; 68-492; 90-847; 95-208; 96-234; 140-178; 72-33;

## 2554: PHENYLETHYL THIOGLYCOLATE

Phenethyl-2-mercapto ethanoate.



$C_{10}H_{12}O_2 = 196.27$

Colorless viscous oil. Sp.Gr. 1.14.

Practically insoluble in water, soluble in alcohol and oils.

Mildly floral-rosy, also sweet-herbaceous odor of moderate tenacity. The odor is strongly influenced by a surplus of one or the other parent component – sulfuraceous or rosy.

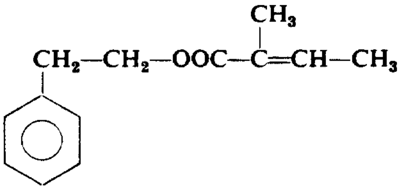
This material may not generally be considered as a fragrance material. It was probably manufactured out of curiosity at the time when Thioglycollic acid became commercially available on a large scale for cold permanent. A few of its esters became available and some are still used in perfumes. However, the title material does not seem to offer any particularly interesting notes to a fragrance.

Prod.: by azeotropic esterification of Phenylethyl alcohol with Thioglycollic acid.

34-1245;

## 2555: PHENYLETHYL TIGLATE

Phenethyl tiglate.
Phenylethyl-*alpha*-methylbutenoate.
Benzyl carbinyl tiglate.



$C_{13}H_{16}O_2 = 204.27$

Colorless, slightly viscous liquid.
Sp.Gr. 1.02. B.P. 259° C.

Practically insoluble in water, soluble in alcohol and oils.

Very pleasant, warm-herbaceous, deep-rosy, dry-leafy-green odor with balsamic-caramellic sweetness and good tenacity.

Sweet and winey, warm-earthy-nutty taste at concentrations below 10 ppm.

This ester has become quite popular since it was made available on a more regular basis about 1960. It had been known and appreciated for a long time, but was not available at a reasonable cost, due to the high cost of Tiglic acid.

It is now used widely in perfume formulations, including soap perfumes as a modifier and fixative/blender in floral and herbaceous fragrance types. It could be compared to Phenylethyl propionate in that it is versatile, warm, floral-herbaceous and very generally useful. With Jasmin or Lilac notes it forms attractive blends, and with Methylionones and Styrax it may form part of a "powdery" undertone in Oriental or "l'Origan"-type fragrance, etc.

The ester is used in flavor compositions partly as a fruity blender/fixative, partly as a modifier in Nut compositions. It blends excellently with Nonanolide, Oakmoss, Hydroquinone dimethylether, etc.

Concentrations are about 1 to 10 ppm in the finished product.

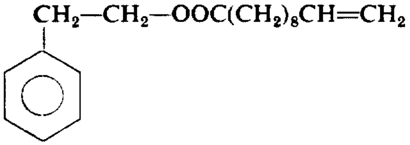
G.R.A.S. F.E.M.A. No.2870.

Prod.: from Phenylethyl alcohol plus Tiglylchloride in the presence of Pyridine catalyst in Benzene solution.

90-341;

## 2556: PHENYLETHYL UNDECYLENATE

Phenethyl undecenoate.



$C_{19}H_{28}O_2 = 288.43$

Colorless or pale straw-colored oily liquid. B.P. near 300° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

Oily-fatty, sweet-Hay-Honey-like, warm-herbaceous odor of considerable tenacity.

This ester, very rarely offered commercially*), is occasionally used in perfume compositions for its Immortelle-like effect in Chypre and Fougère types, and in Jasmin.

Immortelle (St. John's wort, Xeranthemum sp.) has had a lively come-back in perfumery during the past decade, and its effect in Jasmin is highly appreciated. However, there are few chemicals of such odor that they can replace even a part of the natural Immortelle odor.

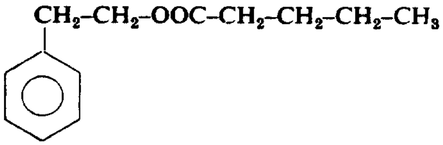
Prod.: by azeotropic esterification of Phenylethyl alcohol with Undecenoic acid.

163-63; 163-371;

*) A material, labelled P.E.B.U. was marketed a few years ago from a perfume material manufacturer. The abbreviation was thanslated "Phenylethyl butyl undecylenate" by the manufacturer, but the name did not correspond to the true identity of the chemical.

## 2557: PHENYLETHYL VALERATE

Phenethyl-*n*-pentanoate.
Benzyl carbinyl valerianate.



$C_{13}H_{18}O_2 = 206.28$

Colorless liquid. B.P. 268° C. Sp.Gr. 0.98.

Practically insoluble in water, soluble in alcohol and oils.

Warm, fruity-rosy, herbaceous-tobacco-like odor of good tenacity.

Sweet, pungent-fruity taste in concentrations below 10 ppm.

This ester finds use in floral and floral-herbaceous fragrance compositions, e. g. Narcisse and Jasmin, and as a modifier for the lower esters in other floral types, including Rose. It is a supporting material in "Tabac" notes with certain types of Oakmoss, Coumarin derivatives or Liatris absolute, *iso*-Butyl quinoline, etc.

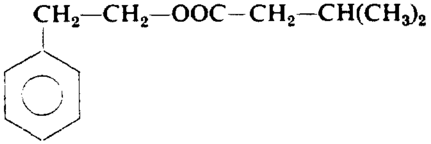
The ester finds some use in flavor compositions for its pleasant modifying effect in Apricot, Apple, Pineapple, Peach, etc. but the *iso*-Valerate (see next) is more commonly used as a flavor material).

Prod.: by azeotropic esterification of Phenylethylalcohol with *n*-Valeric acid.

163-63;

## 2558: PHENYLETHYL-iso-VALERATE

Phenethyl-*iso*-pentanoate.
Benzyl carbinyl-*iso*-valerianate.
Phenylethyl-*3*-methylbutyrate.



$C_{13}H_{18}O_2 = 206.28$

Colorless liquid. Sp.Gr. 0.98. B.P. 263° C.

Practically insoluble in water, soluble in alcohol and oils.

Fruity-rosy, Rose-petal-like, mildly balsamic odor of good tenacity. Not quite as warm-herbaceous as the *n*-Valerate (see previous monograph), but overall fresher, livelier.

Pleasant fruity, fresh-green and sweet taste in concentrations below 10 ppm.

This ester is used more commonly than the *n*-Valerate, but it should not be considered as a replacement or substitute for that ester. The two are sufficiently different that they can be used for different purposes.

The title ester is used in fruity, floral, Oriental, balsamic, Fougère, "Tabac", Rose and other fragrance types in relatively discrete amounts. Concentrations of about 1 to 3% are normally sufficient to achieve a desirable effect, and higher concentrations may often have an adverse effect.

The material is also interesting in "sophisticated" Pine fragrances (i. e. Pine fragrances where the cost limit is considerably higher than the conventional, which only allows for very inexpensive raw materials) because of its "forest-green"-like effect, while it will supply an equally pleasing undertone in floral fragrances.

In flavor compositions, the ester is quite frequently used, mainly in imitation Peach, Apricot, Honey, Pineapple, Apple, Pear, Gooseberry, "tutti-frutti", etc.

Çoncentration is normally as low as 1 to 6 ppm in the finished product.

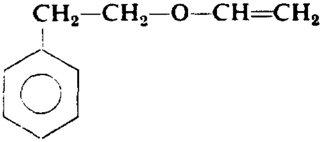
G.R.A.S. F.E.M.A. No.2871.

Prod.: by azeotropic esterification of Phenylethylalcohol with *iso*-Valeric acid.

33-932; 106-301; 156-311; 163-63; 163-311; 5-239;

## 2559: PHENYLETHYL VINYLETHER

*5*-Phenyl-*3*-oxopent-*1*-ene.
Vinyl phenylethyl ether.



$C_{10}H_{12}O = 148.21$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful ethereal-rosy, sweet-pungent odor of moderate to poor tenacity.

This ether has found use in perfumery because of its power and stability in soap. Several ethers of Phenylethylalcohol are used for their exceptional power, but the Methyl- and Ethyl-ethers are more Hyacinth-like pungent and not suitable for Rose compositions in higher concentration.

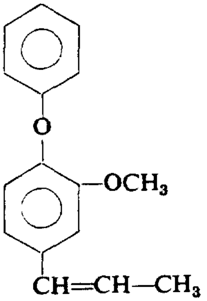
In combination with sweet-balsamic fixatives, Styrax, Cinnamic alcohol, etc. the title ether gives interesting effects, but it needs considerable "blending" to become pleasant and acceptable.

The material is rarely offered commercially, but it may be prepared by various manufacturers of perfume specialties for their own use.

Prod.: from Phenylethyl alcohol and Acetylene under pressure and in the presence of an alkoxide type catalyst.

## 2560: PHENYL-iso-EUGENOL

*iso*-Eugenol phenylether.
Phenyl-*2*-methoxy-*4*-propenylphenylether.



$C_{16}H_{16}O_2 = 240.30$

White crystals.

Insoluble in water, soluble in alcohol (less than 10%), better in hot alcohol and oils.

Very mild, warm-balsamic and sweet odor of excellent tenacity. Poorer grades may show "phenolic" character which is unacceptable and undesirable.

This lower homologue of the more commonly used Benzyl-*iso*-eugenol is occasionally used in perfume compositions for its fixative effect in Carnation, Wallflower, Rose, Lilac and various other floral and floral-balsamic fragrance types. It does not supply much odor of its own, but it will support *iso*-Eugenol, Acet-*iso*-eugenol and other sweet-spicy notes or intensely floral notes. Accompanied by Heliotropine it may contribute to part of the "powdery" and very desirable undertones in such fragrances.

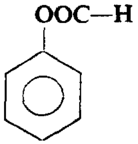
Prod.: from Eugenol plus Potassium hydroxide and Sodium benzene sulfonate, followed by Isomerization of the resulting Phenyleugenol with alcoholic Potassium hydroxide.

NOTE: Phenylethyl-*iso*-eugenol is also a crystalline material and it has occasionally been available. This higher homologue of Benzyl-*iso*-eugenol has, however, not achieved much importance and may be considered as practically obsolete.

There has been some confusion in literature of this material and of the title material.

## 2561: PHENYL FORMATE

This material should not be confused with its empirical isomer, Phenylformic acid, also known as: Benzoic acid.



$C_7H_6O_2 = 122.13$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Pungent, rather sharp, green-herbaceous odor of moderate tenacity.

Although this material has been suggested for use in perfume compositions, there is reason to believe that it is already obsolete or extremely rare in perfumery.

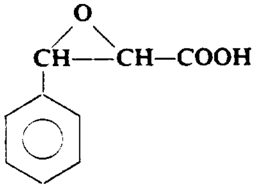
It dos not seem to contribute any interesting or unusual notes, and it inevitably carries a hazard of decomposition into undesirable chemical components, wherefore it would be met with reluctance even if it did bring certain unusual fragrance virtues along.

Prod.: by cold formylation of Phenol.

28-557;

## 2562: beta-PHENYLGLYCIDIC ACID

*alpha-beta*-Epoxy-*beta*-phenylpropionic acid.



$C_9H_8O_3 = 164.16$

White crystals. M.P. 84° C.

Very slightly soluble in water, better in hot water, soluble in alcohol and oils.

Mild, sweet, caramellic-sour odor of considerable tenacity. A highly purified material is said to be virtually odorless.

Although many esters of this acid and its derivatives are used in perfumes and flavors, the acid itself has found only very little application. Its contribution to a fragrance is negligible, and its value as a food acid is very limited.

Briefly, the material has little more than academic interest to the perfumer or the flavorist.

Prod.:

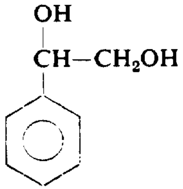
1) from Chloro-hydroxy-*beta*-phenylpropionic acid and alkali.
2) from Cinnamic aldehyde by treatment with alkaline Hydrogen peroxide in the cold.

68-925;

## 2563: PHENYL GLYCOL

*l*-Phenylethanediol-*1:2*.
Monophenyl ethyleneglycol.
"Styrolyl alcohol".
Styrene glycol.

NOTE: The perfume chemical, "Styrallyl alcohol" is Methyl phenyl carbinol (see monograph) and should not be confused with the title material.



$C_8H_{10}O_2 = 138.17$

White amorphous powder. M.P. 68° C.
B.P. 273° C.

Very slightly soluble in water, soluble in alcohol and most perfume oils.

Mild and weak, but sweet and pleasantly floral odor of excellent tenacity.

This glycol has been used in perfume compositions as an auxiliary fixative with modest odorvalue. Its contribution of odor is very limited, and it may be used as supporting note to Gardenia and Lily since it has perceptible traces of that odor character.

Many esters of this glycol are used in perfumery, although a number of them may be considered as practically obsolete today, others are outperformed by esters of Methyl phenyl carbinol, an isomer of Phenylethyl alcohol and known under the name "Styrallyl alcohol" (see above synonyms and NOTE).

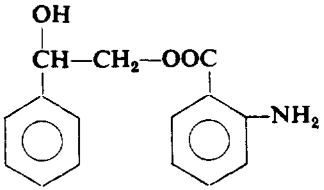
Prod.:

1) from Styrene by oxidation.
2) or from Styrene oxide (epoxide) by hydration.
3) or from Styrene via its Chlorohydrin to the title material.
4) by catalytic hydrogenation of Benzoyl carbinol.

5-61; 31-23; 68-875; 163-64; 163-233; 163-372; See also 1223.

## 2564: PHENYLGLYCOL ANTHRANILATE

"Styrolyl" anthranilate.



$C_{15}H_{15}NO_3 = 257.29$

Colorless viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very faint, sweet-floral, deep-fruity odor with a musty-leafy note.

This ester has been suggested for use in perfume compositions, and it has been available from regular suppliers of perfume chemicals.

However, it seems to be practically obsolete, and there is reason to believe that it has failed to attract interest.

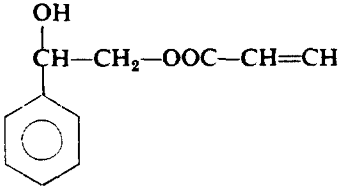
A considerable range of esters of Phenylglycol have been produced but very few have remained commercially available.

The title ester found some use in Honeysuckle, Gardenia and other heavy florals, but it does not contribute very distinctive or attractive notes to those fragrances.

Prod.: from Styrene glycol and Isatoic anhydride.

## 2565: PHENYLGLYCOL CINNAMATE

Phenylethylene glycol monocinnamate (*primary-*).



$C_{17}H_{16}O_3 = 268.32$

White crystals. M.P. 110° C.

Practically insoluble in water, poorly soluble in cold alcohol, better in hot alcohol. Soluble in most perfume oils.

Mild balsamic odor with a faint, but pleasant floral note of Lily-Hyacinth character, and very good tenacity.

The title ester has been suggested for use in perfume compositions as a mildly floral fixative, but it does not present any significant advantage over the conventional materials (Benzyl cinnamate, Phenylethylcinnamate, etc.), nor does it possess any very characteristic or unusual effect from a perfumery point of view.

Briefly, the material is dispensable in perfumery, and may be considered as almost obsolete.

Prod.:

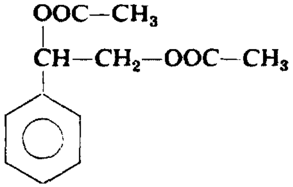
1) from Styrene glycol and Methyl cinnamate by alcohol interchange reaction.
2) by azeotropic esterification of Phenylglycol with Cinnamic acid, preferably in presence of a Toluenesulfonic acid type catalyst.

34-462; 163-233;

## 2566: PHENYLGLYCOL DIACETATE

Phenylethyleneglycol diacetate.
"Styrolyl" diacetate.
"Muguet Principe".
"Gardeniol I".

Note: The material known as "Gardenol" (Givaudan, trade name) is Methyl phenyl carbinyl acetate (see monograph).



$C_{12}H_{14}O_4 = 222.24$

Colorless viscous liquid. Sp.Gr. 1.03.
B.P. 274° C.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant, somewhat heavy, Gardenia-Hyacinth-Lily type odor, more earthy than fruity, and with damp, not truly fresh, greenness. Fair to good tenacity.

The title ester, often confused with "Styrallyl acetate" which is described under the name Methyl phenyl carbinyl acetate in this work, has found some use in perfume compositions for its earthy-green floral-pungent odor and good tenacity. In the latter respect, it is superior to Methyl phenyl carbinyl acetate, but it can not compete with that material in freshness and lively fruity-green power.

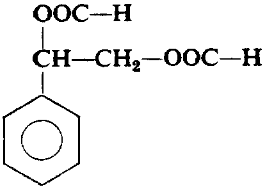
The subject ester is used for Muguet, Lily, Jasmin, Hyacinth, Gardenia and certain other floral fragrance types, and the concentration can be relatively high, since the odor power of this ester is not very great. It performs also well with the Eugenol derivatives in Carnation.

Prod.: from Styrene glycol and Acetic anhydride.

31-504; 163-64; 163-233;

## 2567: PHENYLGLYCOL FORMATE

Phenylethylene glycol di-formate.
"Styrolyl" formate.



$C_{10}H_{10}O_4 = 194.19$

Colorless liquid. B.P. 212° C. Sp.Gr. 1.03.

Insoluble in water, soluble in alcohol and oils.

Fruity-green, rather fresh and powerful odor of moderate to poor tenacity.

Refreshingly green-fruity, Apple-Apricot-like taste in concentrations below 20 ppm. Rather sharp and pungent at concentrations higher than 50 ppm.

This ester is used to a limited extent in perfume compositions, mainly of the Oriental type where a fruity green, mildly balsamic note may be desirable. The effect of this material is in no way unusual or very outstanding, and it can very well be replaced by more interesting, stable and powerful or pleasant chemicals.

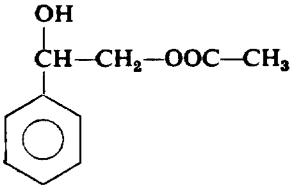
The title ester is also used to a minor degree in flavor compositions, mainly Apple, Apricot, Peach, etc., for its fruity-green, modifying note. Concentrations are normally about 5 to 20 ppm in the finished product, and the material is NOT listed in the American G.R.A.S. list.

Prod.: by cold Formylation of Phenylglycol.

163-64; 163-233;

## 2568: primary-PHENYLGLYCOL MONOACETATE

"Styrolyl" acetate I.



$C_{10}H_{12}O_3 = 180.21$

Colorless, slightly viscous liquid.
Sp.Gr. 1.04. B.P. 217° C.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-green, somewhat pungent, but not harsh, odor of moderate to poor tenacity. Less earthy and less harsh than the odor of the *secondary*-Phenylglycol monoacetate (see next).

This ester has been used for Narcisse and

Hyacinth fragrance compositions and as a modifier in various other powerful floral types.

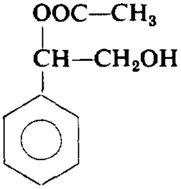
The author is of the opinion that the title material is no longer commonly used, but is more or less obsolete in modern perfumery.

Prod.: by catalytic hydrogenation of Benzoyl carbinyl acetate.

5-61; 7-185; 7-224; 7-341; 33-503; 61-71; 163-233;

## 2569: secondary-PHENYLGLYCOL MONOACETATE

"Styrolyl" acetate II.



$C_{10}H_{12}O_3 = 180.21$

Colorless liquid. Sp.Gr. 1.03.

Very slightly soluble in water, soluble in alcohol and oils.

Harsh-green, also floral and slightly earthy odor of moderate to poor tenacity.

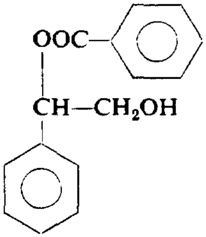
Although this ester has been suggested for use in almost the same types of fragrance as those suggested for its *primary*-isomer (see previous monograph), the title material has failed to maintain a position as a needed perfume chemical.

Occasionally used in Jasmin, Narcisse, Gardenia and similar fragrances, and formerly used in soap perfumes.

7-341; 33-503;

## 2570: PHENYLGLYCOL MONOBENZOATE

Phenylglycol benzoate.
"Styrolyl" benzoate.



$C_{15}H_{14}O_3 = 242.28$

Colorless viscous liquid. B.P. 342° C. Sp.Gr. 1.10.

Insoluble in water, soluble in alcohol and oils.

Mild, balsamic-sweet, dry-floral or woody-floral odor with a delicately green note and excellent tenacity.

The peculiar combination of dry and sweet notes makes this material interesting for experiments with Mimosa, Hyacinth, Acacia, ets.

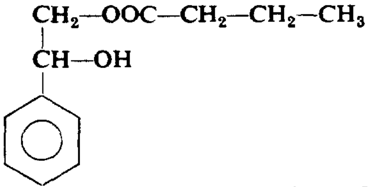
The effect is pleasant, but far too weak to be carried by this material alone. Proper blending with Cinnamic alcohol, Anisyl esters, Methylionone, floral natural materials, etc. is necessary to achieve a reasonable amount of odor effect.

The material is rarely offered commercially, and it is considered practically obsolete in many perfumery circles.

163-233;

## 2571: PHENYLGLYCOL MONOBUTYRATE

*primary*-Phenylethyleneglycol-mono-*n*-butanoate.



$C_{12}H_{16}O_3 = 208.26$

Colorless liquid. Sp.Gr. 1.02. B.P. 231° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet and fruity Lily-Hyacinth-like odor of moderate tenacity. The odor volume is not very great, but the odor type is rather pleasant.

This ester has been used in perfume compositions as a modifier for lower homologues and similar fruity-floral perfume chemicals. The fruity notes are almost Apricot-like with a faint touch of green undertones, while the floral notes are suitable for Lily, Freesia, Magnolia and Sweet Pea.

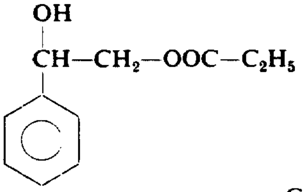
Overall, the material is not very interesting, and it is considered outdated in many perfume laboratories, while a few still find use for it.

Prod.: by catalytic hydrogenation of Benzoyl carbinyl butyrate.

5-62; 7-342; 33-734;

## 2572: PHENYLGLYCOL MONOPROPIONATE

"Styrolyl" propionate I.
Phenylglycol propanoate, *primary-*.



$C_{11}H_{14}O_3 = 194.23$

Colorless liquid. B.P. 223° C. Sp.Gr. 1.03.

Insoluble in water, soluble in alcohol and oils.

Mild, ethereal-fruity, green-floral odor of moderate to poor tenacity, but considerable power.

This ester has occasionally been used in Gardenia, Hyacinth, Narcisse and other powerful floral bases, usually at the rate of a few percent or less in the composition.

The material is not exceedingly interesting, and many perfume laboratories have never had this item on their shelf.

It is used in a number of European perfume houses, but seems to become obsolete gradually in competition with more powerful and inexpensive materials of similar odor type.

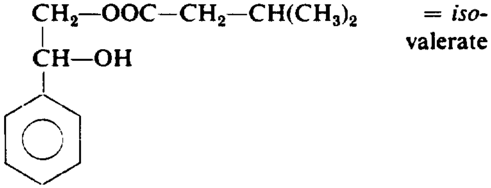
Prod.: by catalytic reduction of Benzoyl carbinyl propionate.

5-62; 7-342; 33-622; 163-233;

## 2573: PHENYLGLYCOL MONO-iso-VALERATE

Phenylethyleneglycol, *primary*-mono-*iso* valerate.

The monograph includes the *n*-Valerate, but the author has preferred to use the *iso*-Valerate as title since it is apparently the most commonly used, if not the only one still in use.



$C_{13}H_{18}O_3 = 222.29$

Colorless oily liquid. B.P. 234° C.
Sp.Gr. 1.03.

Almost insoluble in water, soluble in alcohol and oils.

Relatively powerful and heavy, fruity Gardenia-Narcisse-Hyacinth type of moderate tenacity.

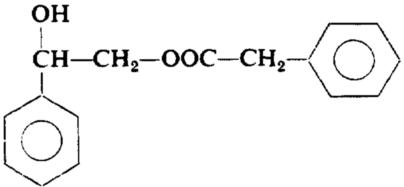
This ester, occasionally used in perfume compositions, serves as a modifier for other fruity-floral perfume chemicals, mostly used in Gardenia and Hyacinth variations. It supplies an ethereal and quite pleasant topnote, but its overall odor value can not compete with the more modern materials, and the title material will most likely vanish from the perfumers' shelves.

Prod.: by catalytic hydrogenation of Benzoyl carbinyl (*iso-*)valerate.

5-62; 7-342; 163-233;

## 2574: PHENYLGLYCOL PHENYLACETATE

Phenylethyleneglycol-*alpha*-toluate.
"Styrolyl"-mono-phenylacetate, *primary*-.



$C_{16}H_{16}O_3 = 256.30$

Colorless, viscous liquid. Sp.Gr. 1.11.
B.P. 340° C.

Insoluble in water, soluble in alcohol and oils.

Heavy and intensely sweet, floral-herbaceous and very tenacious odor of Honey-Gardenia type. The Honey notes may be conspicuous by their absence in the pure material, but they will usually appear upon dilution or in active use of this ester. The floral notes are most perceptible in the undiluted material.

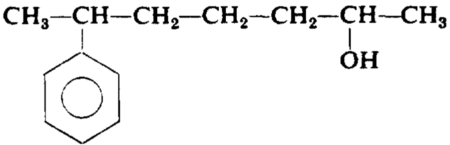
This ester is not often found on the perfume material shelves, and rarely offered commercially. It is still used in certain specialties and older bases, but hardly used in modern creations. Its odor value and overall character are not sufficiently unusual to justify continued use of this ester. Materials of related odor type, e. g. Methyl phenyl carbinyl phenylacetate and Phenylethyl phenylacetate, etc. are being used where the title ester once was intended for use.

Prod.: by catalytic hydrogenation of Benzoyl carbinyl phenylacetate.

34-246; 163-233;
See also monograph 2524.

## 2575: PHENYL HEPTYL ALCOHOL

*6*-Phenyl heptanol-*2*.
NOTE: Although the ambiguous name Phenyl heptyl alcohol is used in perfumery literature, the author believes that reference is almost inevitably made to the *secondary*-alcohol, *6*-Phenylheptanol-*2*.



$C_{13}H_{20}O = 192.30$

Colorless oily liquid. B.P. 261° C.

Almost insoluble in water, soluble in alcohol and oils.

Mild, oily-rosy and delicately green, tenacious odor.

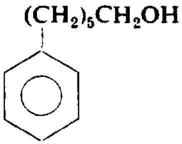
The title alcohol has been suggested for use in perfume compositions as a modifier, mainly in Rose compositions, where it should introduce freshness and discretely green notes. With that odor picture, the title material is also suitable for Muguet, Lily and other delicate, sweet-green florals.

Prod.: from *beta*-Methyl-*beta*-phenylpropionic aldehyde by condensation with Acetone, followed by hydrogenation and reduction to the *secondary*-alcohol.

7-342; 31-23; 163-372;

## 2576: PHENYL HEXYL ALCOHOL

Phenyl-*n*-hexanol.
*1*-Phenylhexanol-*6*. (*primary*).



$C_{12}H_{18}O = 178.28$

Colorless, slightly viscous liquid.
B.P. 258° C.

Almost insoluble in water, soluble in alcohol and oils.

Refreshingly citrusy-green, delicately rosy odor of good tenacity. The odor has sometimes been described as "Rose-Lime"-like, a combination which is rather fashionlable in soap and shaving cream fragrances again.

The alcohol is rarely offered under its proper name, but it is employed in a number of bases and specialties, some of which are several decades old.

It is interesting to follow the odor pattern of the phenylsubstituted alifatic alcohols, and the reader may wish to compare the odor of Phenyl amyl alcohol with those of Phenyl heptyl alcohol and the title alcohol. It is also interesting to note that the sweetest and most pleasant odor appears at Phenyl heptyl alcohol with the formula $C_{13}H_{20}O$ – the same empirical formula as that of the Ionones.

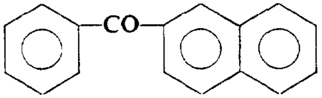
Prod.:
1) from Phenylbutyl magnesiumbromide plus Ethylene oxide.
2) by reduction of Phenylcaproic acid, Ethylester.
3) from Phenylhexyl chloride by treatment with Potassium acetate and Acetic acid, followed by saponification of the ester.

7-342; 31-23;

NOTE: The isomer alcohols:
*2*-Methyl-*2*-phenylpentanol-*4*, and
*1*-Phenylhexanol-*5*, both *secondary*-alcohols, are known to perfumery research.

## 2577: PHENYL NAPHTHYL KETONE

Naphthyl phenyl ketone.



$C_{17}H_{12}O = 232.28$

White crystals.

Insoluble in water, poorly soluble in alcohol, better in hot alcohol, soluble in most oils.

Weak, but very tenacious, floral-Ambre type odor with mildly balsamic notes and variable amounts of Neroli-Orangeblossom notes, according to origin of material.

The title material has been used in perfume compositions as a fixative in low-cost Orange-blossom-Neroli fragrances, mainly for soap.

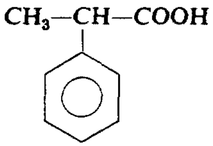
The material has largely been replaced by Methyl naphthyl ketone which is much sweeter and more versatile, although much more expensive, but the cost is compensated for by the power of the material. For lower cost in less refined fragrances, the Methyl- and Ethyl ethers of *beta*-Naphthol are still used quite extensively.

The main difference in the odor picture is that the title material carries a certain amount of Ambregris-like notes, which are not found in the above mentioned, more commonly used crystalline materials.

31-83; 103-274; 163-64;

## 2578: alpha-PHENYLPROPIONIC ACID

Hydratropic acid.
*alpha*-Methyl-*alpha*-toluic acid.
*2*-Phenylpropionic acid (see notes under *3*-Phenylpropionic acid).



$C_9H_{10}O_2 = 150.18$

Colorless liquid. B.P. 265° C. Sp.Gr. 1.09.

Slightly soluble in water, soluble in alcohol and oils.

Heavy-sweet floral Honey-like odor of good tenacity but not very powerful.

This acid has occasionally been used in perfume compositions as supporting note in Honey-bases where the acidity is merely part of the entire aroma picture, while the title material is only rarely used in other fragrance types or perfumes at all. The introduction of acid in a composition is rarely desirable since it inevitably affects the other components, not always in the wanted direction.

Many esters of the acid are used in perfumes and flavors.

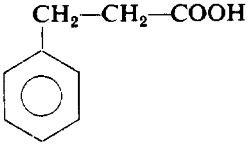
Prod.:

1) from Benzyl cyanide by Methylation with Methyl iodide and Sodamide to produce *alpha*-Phenylpropionitrile, from which the acid is produced by acid hydrolysis.
2) from Acetophenone cyanhydrin with Hydriodic acid.

26-576; 34-582; 68-600; 160-1040; 163-372; B-IX-524;

## 2579: 3-PHENYLPROPIONIC ACID

*3*-Phenyl-*1*-propionic acid.
*gamma*-Phenylpropionic acid.
Hydrocinnamic acid.
Benzene propionic acid.
Benzylacetic acid.
This material is also called:
*beta*-Phenylpropionic acid, but the syllabus "*beta*-" has been abandoned by many chemists in favor of "*gamma*-":



$C_9H_{10}O_2 = 150.18$

Colorless needlelike crystals. M.P. 49° C. B.P. 280° C. Sp.Gr. 1.07 (liquid).

0.6% soluble in water, soluble in alcohol, Propylene glycol, Glycerin and oils.

Very faint, warm-balsamic and sweet odor of Coumarin-Vanillin-type and excellent tenacity.

Mildly acidic, also sweet-Vanilla-Tonka-like taste in concentrations below 20 ppm.

This acid is rarely, if ever, used in perfumes, but it finds some use in flavor compositions, mainly as a fixative in Vanilla imitation, in complexes as a sweetener, and in Cheese imitation flavor for its mild pungency and herbaceous character.

The concentration normally used is equivalent to 0.1 up to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2889.

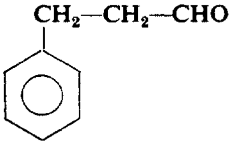
Prod.:

1) by hydrogenation of Cinnamic acid.
2) from Propiophenone and yellow Ammonium sulfide.
3) by acid hydrolysis of *beta*-Phenylethyl cyanide (see 2586).

7-210; 26-576; 68-596; 160-1044; B-IX-508;

## 2580: 3-PHENYLPROPIONIC ALDEHYDE

*3*-Phenyl propanal.
"*beta*"-Phenylpropionaldehyde (somewhat confusing name).
Hydrocinnamaldehyde.
Hydrocinnamic aldehyde.
Dihydrocinnamic aldehyde.
"Phenylone".
Benzyl acetaldehyde.



$C_9H_{10}O = 134.18$

Colorless liquid. Sp.Gr. 1.02. B.P. 222° C.

Very slightly soluble in water, 17% soluble in alcohol, miscible with most oils.

Balsamic-green, oily-earthy odor with warm-spicy undertones and moderate tenacity.

The taste in concentrations below 10 ppm is warm, slightly spicy and sweet with a faint resemblance to Cherry and Bitter Almond.

This aldehyde is used quite commonly in perfume compositions, including soap perfumes. As a modifier in Hyacinth, Rose, Lilac, Heliotrope, Sweet Pea, Frangipanni, etc. or as a novel note in Fougère-spice or Bay-spice odors, it may enter a formulation at the rate of several percent. It does not have the penetrating, pungent power of Phenylacetaldehyde, but it has more of a warm-spicy, deep sweetness, and it is considerably more stable than Phenylacetaldehyde. The aldehyde is of special interest as an undertone in Rose bases.

Traces are used in various berry compositions, Cherry, Almond, Cinnamon, Peach, Plum, etc. to lend a modified and more attractive "Bitter Almond" note than the one supplied by Benzaldehyde alone.

Concentrations in the finished product will be about 1 to 5 ppm.

G.R.A.S. F.E.M.A. No.2887.

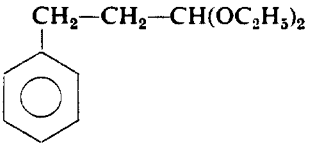
Prod.:

1) from Phenyl propionitrile (Phenylethyl cyanide).
2) from Cinnamic aldehyde diethylacetal by reduction, followed by hydrolysis.

5-110; 26-516; 28-671; 33-158; 34-582; 68-528; 95-138; 96-122; 103-258; 106-307; 156-94;

## 2581: 3-PHENYLPROPIONIC ALDEHYDE DIETHYLACETAL

Hydrocinnamic aldehyde diethylacetal.



$C_{13}H_{20}O_2 = 208.30$

Colorless liquid. B.P. 246° C. Sp.Gr. 1.00.

Practically insoluble in water, soluble in alcohol and oils.

Warm, spicy-floral odor of moderate to good tenacity.

This acetal is rarely offered commercially, but it is sometimes prepared by interested users.

It may find a little use in sweet-floral compositions where discretely spicy notes are desirable, e. g. Carnation, Wallflower, Ylang, Pikake, etc.

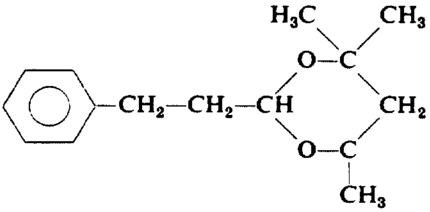
Overall, the acetal has little to offer, and it may well become obsolete without being missed by many.

Prod.: from Hydrocinnamic aldehyde and Formimino diethylether. Also by condensation of the aldehyde with Ethanol in the presence of dry Hydrogen chloride.

37-282;

## 2582: 3-PHENYLPROPIONIC ALDEHYDE-2,4-DIHYDROXY-4-METHYLPENTANE ACETAL

Hydrocinnamic aldehyde-*2,4*-dihydroxy-*4*-methylpentane acetal.
*2*-Phenethyl-*4,4,6*-trimethyl-*1,3*-dioxan.



$C_{15}H_{22}O_2 = 234.34$

Colorless viscous liquid. B.P. 265° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm-floral, tenacious odor with deep-fruity notes and pleasant sweetness.

This acetal has been suggested for use in perfume compositions as a fixative/blender in fruity-floral bases, such as Gardenia, Jasmin, etc.

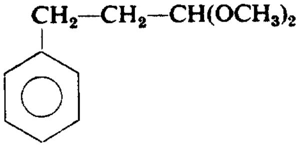
Its odor power is very modest, but its blending ability is of value in compositions with high amount of chemicals.

Prod.: by condensation of Hydrocinnamic aldehyde with *2,4*-Dihydroxy-*4*-methylpentane (a Hexylene glycol).

31-73;

## 2583: 3-PHENYLPROPIONIC ALDEHYDE DIMETHYLACETAL

Hydrocinnamic aldehyde dimethylacetal.
"Dimethylhydrocinnamyle".



$C_{11}H_{16}O_2 = 180.25$

Colorless liquid. B.P. 241° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm, green-floral, sweet and tenacious odor with mildly fruity notes.

This acetal is used in perfume compositions as a modifier in heavy floral and fruity-floral fragrance types. Its contribution is not very unusual in character or in power, and it is most likely that this acetal will become obsolete in perfumery.

Its best areas are in the Sweet Pea type odors, where it can give richness if used in sufficiently high amounts.

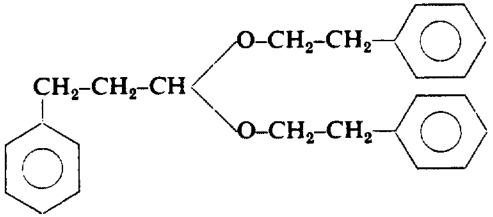
It is also used in Hyacinth, Lilac, Jasmin, Rose, Wallflower, Carnation, etc.

Prod.: by condensation of *3*-Phenylpropionic aldehyde with Methanol in the presence of dry Hydrogen chloride.

5-316; 34-581; 37-282; 163-64;

## 2584: 3-PHENYLPROPIONIC ALDEHYDE DI-PHENYLETHYLACETAL

Hydrocinnamic aldehyde di-phenylethylacetal.



$C_{25}H_{28}O_2 = 360.50$

Colorless, slightly viscous liquid.
Sp.Gr. 1.03.

Practically insoluble in water, soluble in alcohol and oils.

The success of some lower aldehyde acetals with Phenylethylalcohol probably tempted the perfumery research to produce this acetal. However, its odor is rather weak, very sweet, green-rosy and tenacious, overall not very unusual.

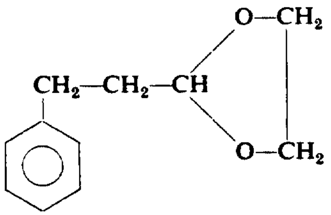
The title acetal has been used in various perfume bases, mainly of the heavy floral, Rose or Oriental types. It was once a component of a successful Rose base.

Prod.: by condensation of Phenylethyl alcohol with Hydrocinnamic aldehyde.

34-581;

## 2585: 3-PHENYLPROPIONIC ALDEHYDE ETHYLENEGLYCOL ACETAL

Hydrocinnamic aldehyde cyclic ethyleneglycolacetal.
*2-beta*-Phenethyl-*1,3*-dioxolan.



$C_{11}H_{14}O_2 = 178.23$

Colorless viscous liquid. B.P. near 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm and very tenacious, floral-fruity odor with sweet-earthy, discretely green notes.

This cyclic acetal was prepared among many related acetals in a research series after the apparent success of the cyclic acetals of Phenylacetaldehyde.

The title acetal is occasionally used in perfume compositions as a fixative/blender in heavy floral, green-floral or Oriental fragrance types. It is particularly useful in rounding-off (blending) the harsher notes in compositions with primarily chemical ingredients.

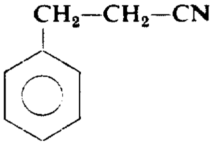
In Gardenia it will blend very pleasantly with Nonalactone, and it is equally suitable with Coumarin in Fougères, etc.

Prod.: by condensation of Hydrocinnamic aldehyde with Ethyleneglycol.

31-73;

## 2586: PHENYL PROPIONITRILE

Hydrocinnamic nitrile.
*beta*-Phenylethyl cyanide.
Phenylpropionic acid, Nitrile.



$C_9H_9N = 131.18$

Colorless liquid. B.P. 261° C. Sp.Gr. 1.00.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and sharp-green, pungent-vegetable type of odor with good tenacity. The odor is more spicy and heavy than that of Benzyl cyanide, although both odors are described as "Watercress"-type odors.

Pungent-green, spicy taste in concentrations near 5 ppm.

The title material is occasionally used in perfume compositions, mainly as a minor ingredient in artificial flower absolutes, etc. It has interesting effect in "Orange flower water absolute" and "Orange leaf water absolute" imitations, particularly in the latter, where the warm-spicy vegetable notes are exceptionally characteristic.

Traces are useful as fresh-green notes in Muguet bases.

The material can also be used in certain types of exotic or very heavy floral fragrance, e. g. Stephanotis, Pikake, Keora, Ginger Lily, Tiare, Coffee flower, etc.

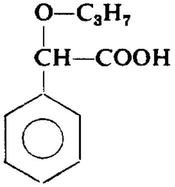
Its warm and piquant, vegetable pungency is utilized in flavor compositions for seasonings, etc. and in various spice blends. The material is not included in the American G.R.A.S. list.

Normal use concentration is equivalent to about 1 to 3 ppm in the finished product.

Prod.:
1) from Phenylethyl bromide plus Sodium cyanide.
2) by distillation of Cinnamic amide with Phosphorous pentoxide under vacuum.

26-578; 68-600; 90-823; 140-175; 163-372; B-IX-512;

## 2587: PHENYL PROPOXYACETIC ACID



$C_{11}H_{14}O_3 = 194.23$

White crystals. M.P. 53° C.

Very slightly soluble in water, soluble in alcohol and oils.

Faint, but very tenacious, oily-balsamic, sweet odor.

This acid has been suggested for use in perfume compositions as a modifier of Phenylacetic acid and higher homologues, but in spite of its milder odor type, almost completely lacking the Honey-theme, it has failed to interest the perfumers in general.

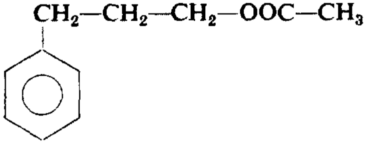
Acids, as such, are not welcome in perfumery except in very specific cases, and unless they possess extraordinary odor characteristics, they are generally avoided in creative perfumery.

The title material could find some use in Rose and Lilac variations, since its effect resembles that of Phenylpropyl alcohol to a certain degree.

31-157;

## 2588: 3-PHENYL PROPYL ACETATE

Hydrocinnamyl acetate.
*beta*-Phenylpropyl acetate (this name is confusing but frequently used in perfumery literature).



$C_6H_5—CH_2—CH_2—CH_2—OOC—CH_3$

$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Sp.Gr. 1.02.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet, floral-fruity, warm and mildly balsamic odor of moderate tenacity.

Pleasant, balsamic-fruity sweet taste in concentrations below 20 ppm.

This ester is used in perfume compositions as a modifier in Hyacinth, Rose, Oriental bases, Lilac and Lily, Reseda, etc. and it blends well with the "rose alcohols", the Linalool family, Styrax and Ylang, Labdanum, Amylsalicylate, etc. Its neutral sweetness makes it very versatile, but it does not lend much odor power to a composition.

Smaller amounts are used in spice flavors, fruit complexes and certain types of berry flavor, including Cherry. The concentration used in such flavors is equivalent to 0.5 to 10 ppm in the functional product.

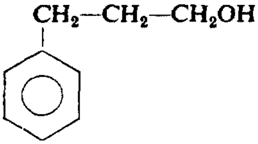
G.R.A.S. F.E.M.A. No.2890.

Prod.: by azeotropic esterification of Phenylpropyl alcohol with Acetic acid.

28-659; 33-503; 34-581; 69-71; 106-305; 140-137;

## 2589: 3-PHENYL PROPYL ALCOHOL

*gamma*-Phenyl-*n*-propylalcohol.
Phenethyl carbinol.
Hydrocinnamic alcohol.
Dihydrocinnamic alcohol.
Benzyl ethyl alcohol.
*3*-Phenyl-*1*-propanol.
*beta*-Phenylpropyl alcohol (this name is frequently used in perfumery literature, but the author finds it confusing and he prefers the name *3*-Phenylpropyl alcohol as title).



$C_6H_5—CH_2—CH_2—CH_2OH$

$C_9H_{12}O = 136.20$

Colorless, slightly oily liquid. B.P. 236° C. Sp.Gr. 1.01.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Warm and mild, balsamic-floral, sweet odor of moderate tenacity. The floral notes have a Lilac-Rose-Hyacinth character, but without the pungency of the Hyacinth, rather the delicate mildness of a Peony.

At concentrations below 10 ppm it has a pleasant, sweet-fruity, balsamic taste reminiscent of fruit preserves and nuts.

This alcohol is widely used in perfume compositions as a blender and modifier of great versatility. It may supply the warm undertone in a Rose, the balsamic sweetness of an Oriental fragrance, or it may form part of the Reseda, Lilac or Cyclamen picture with other floral ingredients. As a variant of Phenylethylalcohol, it may give pleasant modifications.

Small amounts are used in imitation Apricot, Cinnamon, Hazelnut, Peach, Pistacio, Plum, Walnut and other flavor compositions. The concentration will be about 1 to 5 ppm in the finished product.

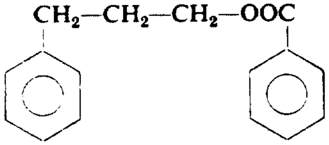
G.R.A.S. F.E.M.A. No.2885.

Prod.: by hydrogenation of Cinnamic alcohol or Cinnamic aldehyde.

34-806; 68-500; 106-306; 156-86; 95-111; 96-91; 5-56; B-VI-503;

## 2590: 3-PHENYL PROPYL BENZOATE

Hydrocinnamyl benzoate.



$C_{16}H_{16}O_2 = 240.30$

Colorless, slightly viscous liquid.

B.P. 338° C. Sp.Gr. 1.05.

Practically insoluble in water, soluble in alcohol and oils.

Very mild, but extremely tenacious, sweet-balsamic, green-herbaceous odor with an almost vegetable type of sweet-green-herbal character.

The title ester is occasionally used in perfume compositions as a fixative and modifier in herbaceous-floral and green-floral fragrance types. It gives interesting undertones if used in liberal amounts in a "l'Origan" type, or with Oakmoss in a "Crêpe de Chine" type, etc.

Its main use, however, is that of a modifying fixative.

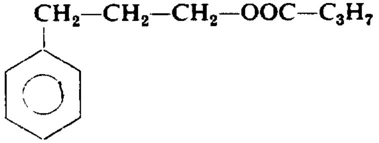
Prod.: from Phenylpropyl alcohol and Methyl benzoate by alcohol interchange reaction.

163-64; 163-234;

## 2591: 3-PHENYL PROPYL BUTYRATE

Hydrocinnamyl-*n*-butyrate.

Sometimes called "*beta*"-Phenylpropyl-butyrate.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid. Sp.Gr. 0.99. B.P. 258° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Heavy, sweet-fruity and balsamic odor of moderate to good tenacity.

Warm, deep-fruity, rather heavy-fruity taste in concentrations near 5 ppm.

This ester finds some use in perfume compositions for Jasmin, Narcisse, Oriental bases, etc. often as a modifier for Benzyl butyrate which it resembles. The title ester is, however, milder and softer.

It is also used in flavor compositions for imitation Apricot and Pineapple, sometimes in Mango.

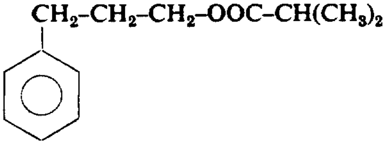
The concentration will normally be mere traces, about 1-5 ppm in the finished product. The material is *not* included in the American G.R.A.S. list, while the *iso*-Butyrate (see next) is included in that list.

Prod.: by azeotropic esterification of Hydrocinnamic alcohol with *n*-Butyric acid.

33-734; 34-581; 163-64; 163-234;

## 2592: 3-PHENYL PROPYL-iso-BUTYRATE

Hydrocinnamyl-*iso*-butyrate.
Sometimes called "*beta*"-Phenylpropyl-*iso*-butyrate.


$CH_2{-}CH_2{-}CH_2{-}OOC{-}CH(CH_3)_2$

$C_{13}H_{18}O_2 = 206.29$

Colorless liquid. Sp.Gr. 0.99. B.P. 252° C.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-balsamic, tenacious, but refreshingly sweet odor. Much fresher than that of the *n*-Butyrate, more refined, less heavy.

This ester finds some use in Jasmin compositions, partly as a modifier for Benzyl-*iso*-butyrate, partly as a supporting note for fruity-balsamic ingredients. It works well with Styrax, which tends to produce a rather "dead" note in floral compositions.

The title ester also finds use in flavor compositions, mainly in imitation Apple, Apricot, Peach, Pear, Pineapple, Plum, Quince, etc. and the concentration used is equivalent to about 1 to 5 ppm in the finished product.

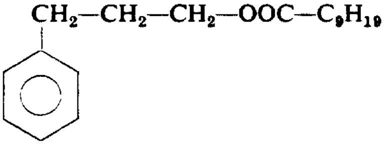
G.R.A.S. F.E.M.A. No.2893.

Prod.: by azeotropic esterification of Hydrocinnamic alcohol with *iso*-Butyric acid.

33-734; 34-583; 163-64; 163-234;

## 2593: 3-PHENYL PROPYL CAPRINATE

Hydrocinnamyl decylate.
"*beta*-"Phenyl propyl decanoate.


$CH_2{-}CH_2{-}CH_2{-}OOC{-}C_9H_{19}$

$C_{19}H_{30}O_2 = 290.45$

Colorless oily liquid. B.P. near 300° C. Sp.Gr. 1.01.

Insoluble in water, soluble in alcohol and oils.

Mild, oily-fruity, slightly green-bland odor reminiscent of unripe Banana, Melon, etc. and with a delicately floral-green undertone. Good tenacity.

Bland, oily-fruity, sweet-green taste in concentrations near 5 ppm.

The author is not aware of any significant use of this ester in perfume compositions.

It is used to a limited degree in flavor compositions, mainly for imitation Banana, Apricot, Pineapple, Peach, etc. and occasionally in Mango. Its tenacity makes it suitable for flavors to be used in hard candy etc. where heat is involved in the processing.

The subject ester is *not* included in the American G.R.A.S. list, and should therefore not be used in flavors in the U.S.A.

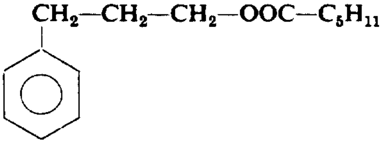
Prod.:

1) from Methyl caprinate and Phenylpropyl alcohol by alcohol interchange reaction.
2) by azeotropic esterification of Phenylpropyl alcohol and *n*-Decanoic acid (Capric acid).

34-583; 163-64; 163-234;

## 2594: 3-PHENYL PROPYL CAPROATE

Hydrocinnamyl hexanoate.
"*beta*-"Phenylpropylhexoate.
Phenyl propyl hexylate.


$CH_2{-}CH_2{-}CH_2{-}OOC{-}C_5H_{11}$

$C_{15}H_{22}O_2 = 234.34$

Colorless liquid. B.P. 292° C. Sp.Gr. 1.01.

Insoluble in water, soluble in alcohol and oils.

Sweet, fruity-green odor of good tenacity.

Warm, rather powerful, fruity taste of Peach-Pineapple-type in concentrations below 10 ppm.

This ester is probably not used in perfumes.

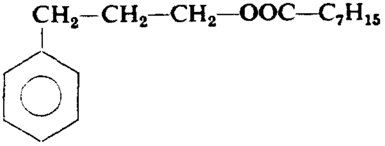
It finds limited use in flavor compositions for Apricot, Pineapple, Melon, Mango, Passionfruit, etc. The concentration used will be about 1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2896.

Prod.: by azeotropic esterification of Phenylpropylalcohol with *n*-Hexanoic acid (Caproic acid).

## 2595: 3-PHENYL PROPYL CAPRYLATE

Hydrocinnamyl octoate.
Phenyl propyl octanoate.
Phenyl propyl octylate.



$C_{17}H_{26}O_2 = 262.40$

Colorless oily liquid. Sp.Gr. 1.01.

B.P. near 300° C.

Insoluble in water, soluble in alcohol and oils.

Sweet, oily-fruity and mildly balsamic odor of excellent tenacity.

Mild, oily-fruity, balsamic taste in concentrations below 5 ppm.

This ester has found some use in perfume compositions, although it is not often offered commercially under its proper name. It is used in specialties and bases as a mellowing and blending agent, a blending fixative with soft and rather versatile odor type.

The author has no report of this ester being used in flavors, but it is most conceivable that it could be used in Banana, Pineapple, Peach and other fruit flavors in concentrations equal to about 1 to 5 ppm in the finished product.

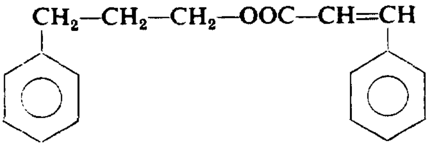
Prod.:

1) from Phenylpropylalcohol and Methyl octoate by alcohol interchange reaction.
2) by azeotropic esterification of Phenylpropylalcohol with *n*-Octanoic acid. (Caprylic acid). See note below.

NOTE: The name "Caprylic acid" is also used commercially for the material: 2-Ethyl hexanoic acid. See monograph: 1263.

## 2596: 3-PHENYL PROPYL CINNAMATE

Hydrocinnamyl cinnamate.
"*beta*-"Phenyl propyl cinnamate.



$C_{18}H_{18}O_2 = 266.34$

Colorless, slightly viscous liquid. Sp.Gr. 1.08
B.P. (under decomposition) over 300° C.

Insoluble in water, soluble in alcohol and oils.

The material polymerizes easily, and becomes insoluble in alcohol, practically odorless and very viscous, hazy or semi-solid.

Very tenacious, rosy-balsamic, delicately fruity odor. Basically mild, but rich and pleasant when pure.

Faintly fruity, sweet-balsamic-oily taste in concentrations below 5 ppm.

This ester is occasionally used in perfume compositions, mainly as a fixative/blender in Mimosa, Rose, Oriental bases, floral and balsamic types, etc. It blends excellently with the Ionones and Methylionones, Labdanum, Castoreum, Styrax, etc. for heavy and lasting fragrances.

It is also used to some extent in flavor compositions, e. g. in imitation Apricot, Butter, Caramel, Chocolate, Cocoa, Coconut, in Grape types, fruit and spice blends, etc.

The concentration used is equivalent to about 1 to 5 ppm in the finished product.

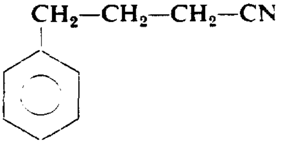
G.R.A.S. F.E.M.A. No.2894.

Prod.: from Phenylpropylalcohol and Methylcinnamate by alcohol interchange reaction.

34-462; 34-583; 90-349; 106-308; 163-64; 163-373; 103-147;

## 2597: 3-PHENYL PROPYL CYANIDE

Phenyl butyro nitrile.
Hydrocinnamyl cyanide.
Phenylbutyric nitrile.



$C_{10}H_{11}N = 145.21$

Colorless mobile liquid. Sp.Gr. 0.99. B.P. 288° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and pungent-herbaceous, deep-green odor of moderate tenacity.

Pungent and heavy-herbaceous-green taste in concentrations below 5 ppm. Burning mouthfeel well below that level. At about 1 ppm the taste is merely pungent-green, yet pleasant and vegetable-like.

This material is used in imitation Horseradish and Radish in flavor compositions for Pickles and other Vinegar-products.

The author does not know of its use in perfume compositions, but it is conceivable that the subject material could be used in artificial flower oils, e. g. Orange flower water oil or in Orange leaf water oil, the so-called Absolue Eaux des Brouts, extracted from the condensation water after distilling Bitter Orange leaves for Petitgrain Bigarade oil.

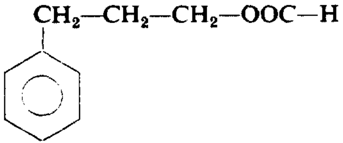
Prod.: from Phenyl propyl chloride and Sodium cyanide.

NOTE: The title material is *not* included in the American G.R.A.S. list, and should therefore be omitted in flavor compositions in the U.S.A.

163-234;

## 2598: 3-PHENYL PROPYL FORMATE

*3*-Phenyl-*1*-propyl methanoate.
Hydrocinnamyl formate.
"*beta*"-Phenyl propyl formate.



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid. Sp.Gr. 1.04. B.P. 238° C.

Almost insoluble in water, soluble in alcohol and oils.

Pleasant, sweet, floral-herbaceous, Geranium-Hyacinth-type odor of moderate tenacity. Its undertones are mildly spicy, warm, cinnamon-like.

Sweet, herbaceous-fruity, quite powerful taste, most pleasant around 5 ppm.

This ester is used in perfume compositions of the heavy-green type, e. g. Hyacinth, Narcissus, etc. and as minor supporting note in Chypre or Oriental bases with Geranium, Styrax, Patchouli etc. Its effect is rather heavy and it needs considerable "blending" with light or fresh odorants in order to perform in a pleasant manner.

Trace amounts are used in imitation red Currant, Raspberry, Apricot, Peach, Honey, in Butter and Caramel compositions and in spicy flavors. The concentration in the finished product will be about 1 to 5 ppm.

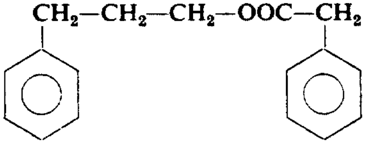
G.R.A.S. F.E.M.A. No.2895.

Prod.: by cold formylation of Phenyl propyl alcohol.

34-581; 106-309; 163-64; 163-234; 103-85;

## 2599: 3-PHENYL PROPYL PHENYLACETATE

Hydrocinnamyl phenylacetate.
Hydrocinnamyl-*alpha*-toluate.
"*beta*-"Phenyl propyl phenylacetate.



$C_{17}H_{18}O_2 = 254.33$

Colorless, slightly viscous liquid.
Sp.Gr. 1.08. B.P. 338° C.

Insoluble in water, soluble in alcohol and oils.

Semi-dry, very heavy, balsamic-spicy and discretely green odor of excellent tenacity. The peculiar dry-sweet topnote resembles the initial notes in Mimosa and Narcisse.

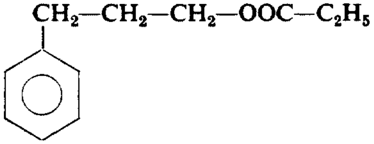
This ester finds some use in perfume formulations as a fixative and blender, mainly in Honeysuckle, Lily, Narcisse, Cassie, Mimosa, Honeybases ("miel") and Oriental fragrance types. It performs very well with the floral carbinols and the Cinnamates, with the "rose alcohols" and the Nitromusks or the Indane musks, etc.

Prod.: by alcohol interchange reaction from Methylphenylacetate and Phenylpropylalcohol.

34-246; 34-583; 163-64; 163-234;

## 2600: 3-PHENYL PROPYL PROPIONATE

"*beta*"-Phenylpropyl propionate.
*3*-Phenylpropyl propanoate.
Hydrocinnamyl propionate.



$C_{12}H_{16}O_2 = 192.26$

Colorless liquid. Sp.Gr. 1.01. B.P. 247° C.

Practically insoluble in water, soluble in alcohol and oils.

Heavy and sweet, but pleasant floral. Lily-Rose-Hyacinth type odor of moderate tenacity.

Sweet and semi-dry-fruity, delicately green taste in concentrations below 5 ppm.

This ester finds a little use in perfume compositions, particularly as part of the Narcisse fragrance picture. It is also used more generally as a sweetener in case that spicy notes are less desirable.

Cinnamic aldehyde and Cinnamylesters are often used as sweeteners, but they carry a certain amount of Cinnamon notes which are not always wanted.

The title ester is also useful in Mimosa compositions with Anisyl acetate, Anisyl alcohol, etc.

Traces are used in imitation Apricot, sometimes as little as 0.5 to 3 ppm in the finished product. It is rarely used in other flavor types

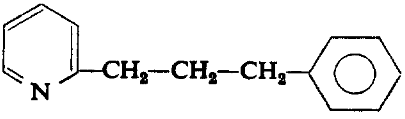
G.R.A.S. F.E.M.A. No.2897.

Prod.: by azeotropic esterification of Phenyl propyl alcohol with Propionic acid.

33-620; 34-581; 163-64;

## 2601: alpha-(3-PHENYL PROPYL)-PYRIDINE

*2*-Hydrocinnamyl pyridine.
*ortho*-Phenylpropyl pyridine.
See NOTE below.



$C_{15}H_{16}N = 210.30$

Colorless oily liquid, straw-colored or pale amber-colored unless freshly prepared.

Insoluble in water, soluble in alcohol and oils.

Powerful, sweet-green and diffusive-floral-woody odor of moderate tenacity. The tenacity of a very pure material is actually poor, while in poorer grade material the residual notes are usually derived from the impurities, and should not be considered characteristic of the material.

This Pyridine (see note below) has been suggested for use in perfume compositions, mainly as a trace ingredient in powerful flower bases, or for "special effects", e. g. to combine with Oakmoss or pyrogenated Styrax in Leather or Tobacco-bases, etc. It is particularly interesting as a trace additive to Ylang and similar products.

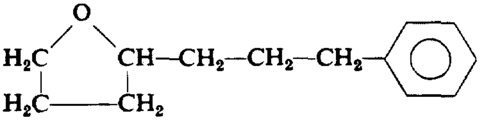
Prod.:

1) by Grignard type reaction upon Pyridine and Phenyl propyl bromide. This method produces *2*- and *4*-isomers.
2) from Phenyl propyl diazoniumchloride plus Pyridine. This method gives all 3 isomers, but mainly the title material.

NOTE: The *4*- or *gamma*-(Phenylpropyl)-pyridine is a commercial item (Reilly Tar & Chemical Co., Inc.) but it has a slightly weaker, less diffusive-green note. It is most conceivable that none of the commercially available materials are absolutely pure.

## 2602: 2-(3-PHENYL PROPYL)-TETRAHYDROFURAN

*alpha*-(*3*-Phenyl propyl)-tetrahydrofuran.
*2*-Hydrocinnamyl tetrahydrofuran.



$C_{13}H_{18}O$ = 190.29

Almost colorless or pale straw-colored liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-caramellic-fruity odor of moderate tenacity.

Honey-like sweet, mildly fruity and caramellic taste in concentrations below 10 ppm.

This material is used in flavor compositions as a sweetener and fruity-caramellic ingredient, mainly in Maple imitation, Nut and Honey flavors, and in various fruit complexes.

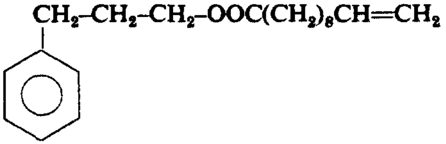
The concentration used is equivalent to about 0.5 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2898.

Prod.: from Furfural via Hydroxymethylfuran and by Grignard reaction to the title material.

## 2603: 3-PHENYL PROPYL UNDECYLENATE

Hydrocinnamyl undecenoate.



$C_{20}H_{30}O_2$ = 302.46

Colorless oily liquid. B.P. near 300° C.
Sp.Gr. 0.95.

Insoluble in water, soluble in alcohol and oils.

Fatty-rosy, heavy, floral and slightly green-herbaceous odor of excellent tenacity.

This rare ester is sometimes used in Chypre or Fougère type fragrances for its tenacity and blending properties. It gives pleasant effects with Amylsalicylate and Oakmoss, and it has a good ability to combine floral notes with the mossy-herbaceous ones.

It is also an interesting variant in Gardenia, and it gives unusually new and pleasant effects with Patchouli and Geranium.

Overall, a material which invites to experiments, if it is at all available.

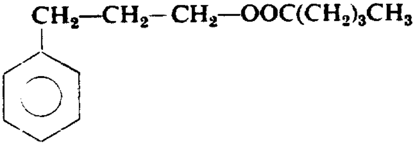
Prod.:

1) from Methyl undecenoate and Phenyl propyl alcohol by alcohol interchange reaction.
2) by azeotropic esterification of Phenyl propyl alcohol with Undecylenic acid.

163-373;

## 2604: 3-PHENYL PROPYL VALERATE

Hydrocinnamyl-*n*-valerate.
*3*-Phenyl propyl-*n*-pentanoate.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid. Sp.Gr. 1.02. B.P. 285° C.

Practically insoluble in water, soluble in alcohol and oils.

Heavy-fruity, mildly spicy-balsamic, deep-sweet odor of good tenacity. The fruity notes are rather fruit-preserve-like, reminiscent of Raspberry-Strawberry jams.

This ester may find a little use in perfume compositions, but its main use is in flavors. Its very deep-sweet, fruity-marmelade-like taste is appreciated in imitation Strawberry and Raspberry for hard candy etc., where the stability and fixative effect of the title material come in handy. The title material is not included in the American G.R.A.S. list, but the *iso*-Valerate is, see next monograph.

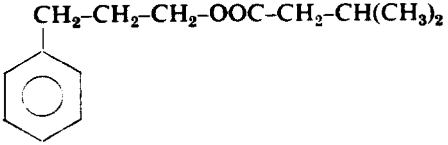
The concentration used will normally be equivalent to about 1 to 5 ppm in the finished product.

Prod.: by azeotropic esterification of Phenylpropyl alcohol with *n*-Valeric acid.

33-933; 34-582; 163-65; 163-234;

## 2605: 3-PHENYL PROPYL-iso-VALERATE

Hydrocinnamyl-*iso*-valerianate.
*3*-Phenyl propyl-*beta*-methylbutyrate.
NOTE: The name "Phenyl propyl valerate" is also used for this item. See previous monograph.



$C_{14}H_{20}O_2 = 220.31$

Colorless liquid. Sp.Gr. 1.00. B.P. 280° C.

Practically insoluble in water, soluble in alcohol and oils.

Distinctly fruity, refreshing and Strawberry-Prune-Plum-like, very sweet and tenacious odor.

Sweet, marmelade-like, "cooked" fruity taste, with mildly nut-like undertones in concentrations near 5 ppm.

The title ester may be used in perfumes, but only to a very limited extent.

It is used in flavor compositions for imitation Butter, Caramel, Nut, Apple, Pear, Plum, Prune, Strawberry, etc. partly as a fixative for the more volatile esters, partly to introduce the "fruit-preserve" like taste, or the mildly oily taste for Nut or Butter aromas.

The concentration is normally about 1 to 2 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2899.

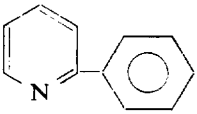
The *n*-Valerate (see previous monograph) is not mentioned specifically in the G.R.A.S. list, but it is reasonable to assume, that the names are used quite indiscriminately in the flavor trade, and that both esters are used in flavors.

Prod.: by azeotropic esterification of Phenylpropyl alcohol with *iso*-Valeric acid.

33-934; 34-583; 163-64; 163-234;

## 2606: alpha-PHENYL PYRIDINE

*2*-Phenyl pyridine.



$C_{11}H_9N = 155.20$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm, pungent-floral, mildly green odor of moderate to poor tenacity. A material which is not absolutely pure, may show unpleasant terminal notes, not characteristic of the title material. Basically it is a topnote-material and it should not reach further than the middle notes in a composition. It is therefore very important that the material is absolutely free from impurities, and particularly free from high-boiling residues.

The title material has found a little use in heavy and exotic type floral fragrances or flower bases, specialties, etc. It will enter a perfume composition at concentrations varying from 0.1 to 0.5%, but it is quite common that the concentration becomes much lower when the perfume(base) is eventually incorporated into a final fragrance, which, of course, is further diluted in the functional product. Under such circumstances, there is apparently no general reluctance in using this and related Pyridines in fragrances.

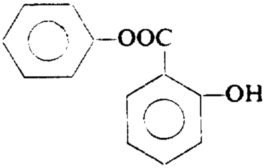
Prod.: from Benzene diazonium chloride plus Pyridine at 30° C. This process yields mainly the *ortho*-isomer.

NOTE: *gamma*- or *4*-Phenyl pyridine is also used in perfume compositions.

68-549; 69-526; 163-373;

## 2607: PHENYL SALICYLATE

Salol.
Phenyl-*ortho*-hydroxybenzoate.



$C_{13}H_{10}O_3 = 214.22$

White granular crystals. M.P. 43° C.
B.P. 282° C. Sp.Gr. 1.25 (liquid).

Almost insoluble in cold water, slightly soluble in hot water, 17% soluble in alcohol, 10% in mineral oil, soluble in most perfume and flavor materials.

Very mild and sweet, fruity-balsamic odor, like very subdued Wintergreen, also reminiscent of Benzyl salicylate, but not as floral. Impure material usually carries a phenolic note, overriding all sweet and pleasant notes.

Sweet, mildly medicinal taste at concentrations near 50 ppm. The medicinal taste is most conceivably derived from hydrolyzed ester.

This material, a common pharmaceutical chemical and mild bactericide, is rarely, if ever, used for its fragrance or flavor, but it may enter certain functional products (dentifrice preparations) as such high level, that its flavor heavily influences the actual flavor composition in its aromatic effect.

It it therefore interesting to study the flavor of the title material if it will be used in a mouthwash, toothpaste or other oral preparation (it was once used as a sunscreening agent).

Fortunately, the flavor of the title ester is not an offensive one, and it will blend very well with the most common types of oral preparation flavors: Peppermint – Spearmint (not so good, however), Wintergreen (excellent), Cinnamon (good) and other spice (good).

Certain concentrated mouthfreshener drops contain more than 5% Salol, and this may be considerably more than the flavor itself. If the Salol is of impeccable quality, there is no problem.

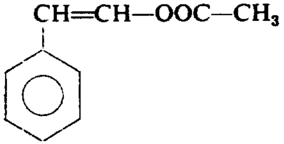
Salol forms liquid physical mixtures with a number of common crystalline materials: Camphor, Menthol, Thymol, etc.

Prod.: from Salicylic acid by heating at 200–220° C. Also from Salicylic acid and phenol with Phosphorous oxychloride among other methods.

34-789; 68-760; 100-805; 160-1220; 163-234; B-X-76;

## 2608: PHENYL VINYL ACETATE

*beta*-Phenyl vinyl acetate.
Styryl acetate.
Vinyl phenyl acetate.
The commercial material is normally a mixture of *cis*- and *trans*-isomers.



$C_{10}H_{10}O_2 = 162.19$

The pure *cis*-isomer is a solid. M.P. 33° C. The pure *trans*-isomer is a colorless or pale straw-colored viscous liquid. B.P. 230° C.

The commercial material is usually a viscous liquid.

Intensely sweet, but also pungent, heavy, Honey-like odor of moderate to good tenacity.

This material, which is rarely offered under its proper chemical name, is used in perfume compositions and bases as a major component in "miel" (Honey) bases and in other specialties.

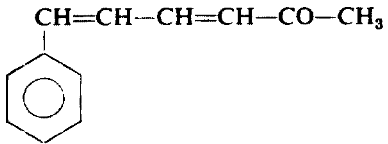
It has an excellent effect in Mimosa and Cassie bases, and it gives very intriguing notes with Oakmoss products.

If one must mention a drawback of this material, it would be the fact that it is sensitive to moisture and it will produce Phenylacetaldehyde upon hydrolysis. This will severely influence the odor picture of the title material.

68-981; 31-125;
(see also: Paul Z. Bedoukian: Journal of the American Chemical Society, 1944, vol. 66, page 1325).

## 2609: PHENYL VINYLETHYLENE METHYLKETONE

Cinnamylidene acetone.
Phenyl-*1*,*3*-butadiene methylketone.
*6*-Phenyl-*3*,*5*-hexadien-*2*-one.
*1*-Phenylhexa-*1*,*3*-dien-*5*-one.
Chrystanthone.
Note: This material is *not* identical to the "Chrysanthone" identified as component of Chrysanthemum (plant).



$C_{12}H_{12}O = 172.23$

White crystals. M.P. 68° C.

Practically insoluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and most oils.

Warm-herbaceous, green-floral and very tenacious odor.

This material, rarely offered under its proper name, and often confused with the natural component of Chrysanthemum, is occasionally used as a fixative and floral-herbaceous blender/modifier in perfume compositions.

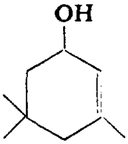
Although it seems to be absolutely unknown in many perfumery circles, it is very highly appreciated by others, and it can give quite unique effects when used with experience. It gives very pleasant notes with Mimosa absolute, Ylang, Opopanax, Patchouli, etc. in the heavy Oriental-floral type.

Prod.: by condensation of Cinnamic aldehyde with Acetone.

36-1255; 68-990; 103-274; 163-65;

## **2610:** iso-**PHOROL**

*3,5,5*-Trimethyl-*2*-cyclohexen-*1*-ol.



$C_9H_{16}O = 140.23$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm and sweet-herbaceous, honey-like odor. Although the odor does resemble that of *iso*-Phorone (see next) to a minor degree, it is much softer and sweeter, and does not have the harsh, pungent and agressive topnote as found in *iso*-Phorone.

This alcohol has found a little use in perfume compositions, mainly in Honey-bases as a modifier and powerful ingredient. It blends excellently with Phenylacetic acid and its esters, with Mimosa, Labdanum and the conventional Acetophenone-derivatives, and it is, incidentally, very interesting in Ylang-Ylang.

Prod.: (several methods) e. g. from *iso*-Phorone by controlled hydrogenation. It has also been prepared from *3,3*-Dimethyl cyclohexanol.

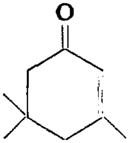
Catalytic hydrogenation of *iso*-Phorone yields Dihydro-*iso*-phorone, see that monograph.

It is also interesting to note that complete hydrogenation (or hydrogenation of the title material, further) yields *3,5,5*-Trimethyl cyclohexanol, which is known under the name Cyclonol, and is used as a technical substitute for menthol.

See monographs:
Dihydro-*iso*-phorone. (967).
*iso*-Phorone. (2611).
*3,5,5*-Trimethyl cyclohexanol. (2998).

## **2611:** iso-**PHORONE**

*3,5,5*-Trimethyl-*2*-cyclohexen-*1*-one.
*iso*-Acetophorone.



$C_9H_{14}O = 138.21$

Colorless liquid. The commercial material is often pale straw-colored. B.P. 202° C.

Almost insoluble in water, soluble in alcohol and oils.

Pungent, sweet-camphoraceous, heavy odor of poor tenacity. In extreme dilution, the odor is less camphor-like, more honey-like and sweet, yet heavy.

This ketone, manufactured on a very large scale in the Petrochemical industry, is occasionally used in perfumery as a masking agent or odorant with special effects. Curiously enough, the perfumer may occasionally face the problem that a customer wants to have a perfume with which he can mask the odor of *iso*-Phorone, e. g. in a plant where the ketone is used as a solvent (rubber-industry, etc.) and the vapors seem to annoy the employees.

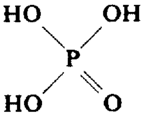
In low-cost Lavender-Fougère types it works well with Coumarin and Amylsalicylate, and it can also be used in conjunction with the Pine chemicals of the Cyclohexanone family. Generally, it will give power and "lift" to these fragrances, and it is quite useful in the modern "heavy-duty" type of liquid detergents, cleansers, etc.

Prod.: from Mesityloxide and Ethylacetoacetate by condensation, followed by hydrolysis and decarboxylation.

67-210;
see also monographs:
Dihydro-*iso*-phorone. (967).
*iso*-Phorol. (2610).
*3,5,5*-Trimethyl cyclohexanol. (2998).

## 2612: PHOSPHORIC ACID

*ortho*-Phosphoric acid.



$H_3PO_4 = 98.00$

The commercial material is a syrupy liquid. Sp.Gr. 1.87. B.P. 261° C. Very pure, anhydrous Phosphoric acid is a colorless crystalline material of M.P. 42° C. It is very hygroscopic and normally handled in the syrupy (not anhydrous) state.

Miscible with water, soluble in alcohol and in many oils.

Practically odorless. Aqueous solutions of concentration near or below 500 ppm have a sharp acid taste.

This acid is sometimes preferred over citric acid as a food acid because it produces a "quick-sharp" acidity or taste impression. This is particularly desirable in Cola-type carbonated beverages.

The Cola-type is the soft drink of the lowest $p_H$ of all carbonated beverages. The $p_H$ is about 2.4 which is lower than in most brands of Pickle Vinegar.

The Cola type beverage is furthermore the type with the highest carbonation, often about 3.5 volumes $CO_2$.

As a special advantage. Phosphoric acid can claim the position as the most inexpensive of all food acidulants. However, its use in foods is confined to carbonated beverages and a few types of candy.

The concentration used is about 500 ppm in carbonated beverages and up to 5000 ppm in candy.

The acid is also used in Cheese and Beer as a $p_H$-adjusting acid.

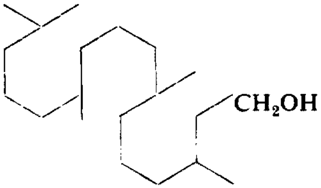
G.R.A.S. F.E.M.A. No.2900.

Prod.: from natural crude Tricalcium phosphate and Sulfuric acid.

100-908; 160-620; 161-319;

## 2613: PHYTOL

*3,7,11,15*-Tetramethyl-*2*-hexadecen-*1*-ol.
Hexahydro-geranyl geraniol (sometimes called).
A member of the chemical synthesis of Vitamin E.



$C_{20}H_{40}O = 296.54$

Practically colorless, viscous liquid.
Sp.Gr. 0.85. B.P. over 310° C.

Insoluble in water, miscible with alcohol and oils.

To most observers, this material is odorless and tasteless. And for those who have heard much interesting about the material, the first meeting is probably a disappointment. On a closer study, one may detect very delicate, floral-balsamic notes, resembling those of Nerolidol and Farnesol. These could, however, very well be uncharacteristic of the pure Phytol itself, and carried over in the chemical process.

Phytol was for many years a material the perfumer would read about but not have in his laboratory, and probably not even wish to have in his laboratory. Except for a few curious or agressive perfumers.

The material has now been made commercially available at a very attractive price, and many perfumers feel that there is no excuse for not at least trying it. To this comes the information through modern instrumental analysis, that the material may be an important component in several highly appreciated flower absolutes, and actually be quite widely distributed in Nature.

It is hard to describe the odor of this material in words such as "virtually odorless but of outstanding tenacity", yet this would be briefly what is true about Phytol. Or, in more scientific words, it has an unusually low vapor pressure at normal temperature, and is therefore an excellent fixateur. There is good reason to try it in a composition. And it has been tried in artificial flower absolutes with success.

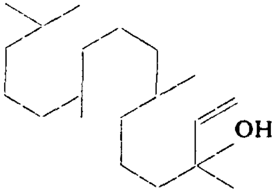
Prod.:

1) by isolation from the Chlorophyll-extract (e. g. from Alfalfa grass) by decomposition.
2) from Farnesol via Hexahydrofarnesylbromide to *2,6,10*-Trimethylpentadecanone-*14* and to Phytol by Ethinylation and selective hydrogenation.

67-713; 88-360; 100-815; 160-1168; 163-65; 163-234; 163-373; B-I-453;
Material and additional data: Hoffmann-laRoche, Inc. Nutley, N. J. (U.S.A.).

## 2614: iso-**PHYTOL**

*3,7,11,15*-Tetramethylhexadecen-*1*-ol-*3*.
Hexahydro geranyllinalool (sometimes called).
An alcohol closely related to synthetic Vitamin E.



$C_{20}H_{40}O = 296.54$

Practically colorless viscous liquid.
Sp.Gr. 0.84. B.P. over 310° C.

Insoluble in water, soluble in alcohol and oils.

The alcohol will form salts with certain acids.

Virtually odorless and tasteless when absolutely pure, but normally carries a delicate, dry-leaf, tea-like and slightly caramellic-sweet odor.

This material was available at a relatively low price earlier than Phytol itself, and therefore was introduced to the perfumers as a natural flower oil fixative. However, there has been some differences of opinion as to the advantage of Phytol over *iso*-Phytol.

Certain types of *iso*-Phytol were brought on the market in a state of deplorable impurity, occasionally with Sulfide by-notes, or other undesirable, very perceptible notes. There is reason to believe that a high-grade *iso*-Phytol is a useful and effective material for application in artificial flower absolutes, and in certain perfume bases, specialties, etc.

If Phytol is available at the same price as *iso*-Phytol, there is reason to believe that Phytol will be the preferred item, because it was first mentioned in connection with flower oils, and it had an advance reputation. It is extremely difficult to demonstrate the actual difference in perfumery effect between the two materials.

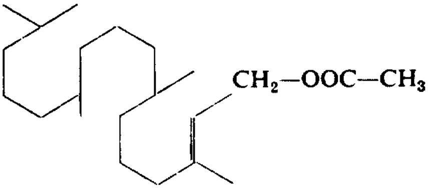
Prod.:

1) by decomposition of Chlorophyll extract from Alfalfa grass.
2) by hydrogenation of Geranyl linalool (see monograph).

88-360; 100-578; 163-350;

## 2615: PHYTYL ACETATE

*3,7,11,15*-Tetramethyl-*2*-hexadecen-*1*-yl acetate.
(See also Phytol).



$C_{22}H_{42}O_2 = 338.58$

Colorless, slightly viscous liquid.
B.P. over 310° C.

Insoluble in water, soluble in alcohol and oils.

Faint, but pleasant and discretely fruity-acidulous odor of excellent tenacity. There is a trace of floral-balsamic note combining with the fruity note to a pleasing fragrance.

Both Phytol and *iso*-Phytol may carry faint odors, but the odor is usually only brought up in actual "use" and dilution.

The title ester has been made commercially available a few years ago by a company in the Vitamin industry. The ester could serve as a supporting fixative in floral bases, artificial flower absolutes, etc. It will introduce a delicate, fresh note useful in Muguet types, Ylang, Jasmin, Tuberose, Rose and many other florals, but its value is at times difficult to estimate, particularly when it is used in combination with powerful odorants.

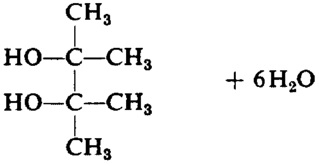
At the present, relatively low cost of this ester, there is reason to believe that it will find firm places in creative perfumery, as more perfumers realize the olfactory value and "finesse" of the subject material. It takes considerable experimenting to become convinced of its effect.

Prod.: from Phytol and Acetic anhydride with a Pyridine type catalyst.

88-362;
(material: Hoffmann-laRoche, Inc.).

## 2616: PINACOL

Tetramethyl ethyleneglycol.
*2,3*-Dimethyl-*2,3*-butanediol.
Pinacol is a general term for *1:2*-Glycols with *secondary*- or *tertiary*-alcohol groups.



$$\begin{array}{l} \quad CH_3 \\ \quad | \\ HO-C-CH_3 \\ \quad | \\ HO-C-CH_3 \\ \quad | \\ \quad CH_3 \end{array} \quad + 6H_2O$$

$C_6H_{14}O_2 = 118.17\ (+\ 6\ H_2O)$

The material usually crystallizes with 6 Mol. water.

Colorless crystal needles. M.P. 41° C. (45° C. when anhydrous). B.P. 174° C.

Sp.Gr. 0.97 (liquid).

Slightly soluble in cold water, soluble in hot water, alcohol and oils.

Powerful, sweet, bread-like, honey-like, diffusive odor of poor tenacity. Although the impression is that of a warm, aromatic and sweet odor, there is an overall "chemical" odor to the commercial product.

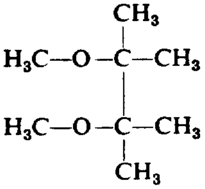
The subject glycol has been used at times in perfume compositions for industrial masking purposes, often for masking problems in which *iso*-Phorone is also used, masking of solvent odors, etc. Its solubility in water is sometimes an advantage.

Prod.: by reduction of Acetone.

66-659; 100-820; 160-1170; B-I-487;

## 2617: PINACOL DIMETHYLETHER

*2,3*-Dimethyl-*2,3*-butanediol dimethylether.
Tetramethyl ethyleneglycol dimethylether.



$$\begin{array}{l} \qquad\quad CH_3 \\ \qquad\quad | \\ H_3C-O-C-CH_3 \\ \qquad\quad | \\ H_3C-O-C-CH_3 \\ \qquad\quad | \\ \qquad\quad CH_3 \end{array}$$

$C_8H_{18}O_2 = 146.23$

Colorless liquid. B.P. 144° C.

Slightly soluble in water, soluble in alcohol and oils.

Warm, sweet and rather pleasant, herbaceous-caramellic odor of poor tenacity.

This glycolether is occasionally used in perfume compositions as part of masking odors for industrial purposes. Its odor is not quite as harsh or pungent as that of Pinacol itself, but it is equally diffusive, and may often distract undesirable odors sufficiently that an acceptable masking effect is achieved.

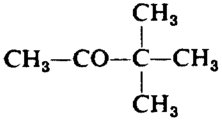
It is no longer commonly used for these purposes, since many new chemicals, including such materials that were "rejected" as fragrance chemicals out of perfume chemical research, are being used for various masking purposes with greater effect. But since the title material is a volume-produced, industrial chemical, it is available at low cost.

Prod.: from Pinacol by Methylation.

100-820;

## 2618: PINACOLONE

Pinacone.
Pinacolin (old name).
*3,3*-Dimethyl-*2*-butanone.
*tertiary*-Butyl methyl ketone.
Methyl-*tertiary*-butyl ketone.
*2,2*-Dimethylbutan-*3*-one.



$$\begin{array}{l} \qquad\qquad\quad CH_3 \\ \qquad\qquad\quad | \\ CH_3-CO-C-CH_3 \\ \qquad\qquad\quad | \\ \qquad\qquad\quad CH_3 \end{array}$$

$C_6H_{12}O = 100.16$

Colorless liquid. Sp.Gr. 0.73. B.P. 106° C.

2.5% soluble in water, 2.5% soluble in alcohol, soluble in some oils, poorly soluble in most other oils.

Powerful and diffusive, ethereal-minty-camphoraceous, warm-sweet odor of poor tenacity. There is some resemblance to the odor of *iso*-Phorone.

This ketone has sometimes been used as masking agent in fragrances for industrial masking. Its solubility in water is sufficient to give it some advantage over the conventional fragrance chemicals, but its poor solubility in alcohol and oils are disadvantages against the use of this material, when many powerful, low-cost fragrance chemicals are available.

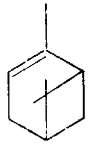
Prod.:

1) by distillation of Pinacolhydrate with diluted Sulfuric acid.
2) from Pinacol dimethylether by heating with Boron trioxide at 140° C.

31-91; 100-820;

## 2619: alpha-PINENE

Dihydro-*para*-cymene (old, confusing name).
*2*-Pinene.
*2,6,6*-Trimethyl bicyclo-(*3,1,1*)-*2*-heptene.
Commercial Pinene with high *alpha*-isomer content is also sold under various trade names.



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 157° C.

Practically insoluble in water, soluble in alcohol (not in diluted alcohol) and miscible with most perfume oils. Almost insoluble in Propylene glycol and Glycerin. It is flammable, but its flashpoint is higher than ordinary room temperature, and the material does not carry explosion hazard.

*alpha*-Pinene is one of the lowest boiling of all Monoterpenes, and has therefore the most diffusive odor and poorest tenacity. It is also one of the purest commercially available Monoterpenes, the chief impurities being *beta*-Pinene and Camphene.

Its odor is warm-resinous, refreshing Pine-like, but lower grades of this material may carry more pronounced "Turpentine"-like odor, "Rosin"-odor or even herbaceous-aromatic odor (common feature of autoxidized *alpha*-Pinene).

The material as such is not a very important perfume chemical. Apart from use in artificial Pine needle oil or fragrance, it will only be a minor ingredient in other compositions: artificial Lemon, Bergamot, Nutmeg, Geranium, Lavandin, etc. and for these particular purposes, the *alpha*-Pinene must be of high olfactory purity.

Thousands of tons are used (mainly in Europe) as starting material in the manufacture of Terpineol, while this alcohol in the U.S.A. is mainly produced as an isolate from steam distilled Pine (stump) oil. European Turpentine is particularly rich in *alpha*-Pinene (mostly *laevo*-rotatory, except Greek, which is *dextro*-rotatory), while American Turpentine has a considerable amount of *beta*-Pinene. The *alpha*-Pinene in American Turpentine is *dextro*-rotatory.

The title material is also used in flavor compositions, partly as ingredient in artificial Lemon and Nutmeg oils, partly as component of such type flavors. The concentration in the finished product will be about 15 to 150 ppm. *alpha*-Pinene has a more balsamic taste, while *beta*-Pinene, less suitable for flavors, has a dry-woody character.

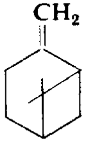
G.R.A.S. F.E.M.A. No.2902.

Prod.: by fractionation of Sulfate Turpentine or neutral Turpentine. It has also been made by isomerization of *beta*-Pinene.

87-127; 100-820; 160-1170; 163-65; 163-234; 163-373; 85-98;
Arizona Chemical Co. – data sheet, samples.
Hercules Powder Co. – data sheet, samples
Glidden-Durkee Co., samples & info.

## 2620: beta-PINENE

Nopinene.
*2(10)*-Pinene.
Commercial *beta*-Pinene contains 85-90% *beta*-Pinene with *alpha*-Pinene as the main impurity. Smaller amounts of Myrcene and Dipentene are also present.
Better grades of *beta*-Pinene contain about 96% *beta*-Pinene and only about 1% *alpha*-Pinene.



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. B.P. 166° C.
Sp.Gr. 0.87.

Insoluble in water, soluble in alcohol (the solubility in diluted alcohol is slightly better than that of *alpha*-Pinene). Soluble in oils, almost insoluble in Propylene glycol and Glycerin.

Dry-woody, resinous-piney odor of poor tenacity.

This Terpene is not used to any great extent as such in perfumes or flavors. As a chemical starting material or intermediate, it is one of the most important of all chemicals in the perfume industry. Via its pyrolysis-product, Myrcene, it opens the way to chemical synthesis of countless large-volume, every-day used fragrance and flavor chemicals: Citral, Citronellal, Hydroxycitronellal, Geraniol, Citronellol, Linalool, Ionones, Methylionones, Menthol, etc. etc.

Smaller amounts are used in the reconstruction of (artificial) essential oils, e. g. Lemon and Nutmeg oils.

The concentration used in flavors is equivalent to about 15 to 600 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2903.

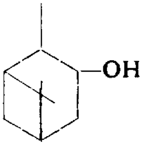
Prod.:

1) by isolation from American Turpentine (minor component).
2) it is also possible to convert *alpha*-Pinene into *beta*-isomer.

65-62; 87-164; 163-234; 163-373;
Arizona Chemical Co. data sheet.
Glidden-Durkee Co., samples & info.

## 2621: dextro-**PINOCAMPHEOL**

*2,6,6*-Trimethyl-*1,3,3*-bicycloheptanol-*3*.
*3*-Pinanol.
Four stereo-isomeric Pinocampheols are known.



$C_{10}H_{18}O = 154.24$

White crystals.
M.P. 67° C. (*dextro-*).
M.P. 57° C. (*dextro-iso-*).
B.P. 217° C. (*dextro-*).
Sp.Gr. 0.97.

Practically insoluble in water, soluble in alcohol and oils.

Fresh, Camphor-Menthol type odor of moderate to poor tenacity. The *dextro-iso-*isomer has a more dry, Borneol-woody odor.

The title material is the most desirable from an olfactory point of view.

This bicyclic terpene, which is an isomer of Dihydromyrtenol, has occasionally been available commercially in very large quantities, and therefore subject to some interest from the perfume industry, particularly with soap and detergent fragrances in mind.

Its odor is quite suitable for modern type detergents as a departure from the straight Pine or the medicated Rosemary-type. It has more fresh lift, and it can be modified into a sweeter fragrance with proper additives.

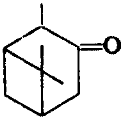
Prod.:

1) by reduction of Pinocamphone or Pinocarvone with Sodium and alcohol.
2) by catalytic hydrogenation of Pinocarveol (see monograph), which is obtainable from *beta*-Pinene.

67-568; 65-237; 88-138; 163-373;

## 2622: PINOCAMPHONE

*2,6,6*-Trimethyl-*1,3,3*-bicycloheptanone-*3*.
*3*-Pinanone.



$C_{10}H_{16}O = 152.24$

Colorless or very pale yellowish oily liquid.
B.P. 212° C. Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils.

Warm-camphoraceous, Cedarleaf-like, slightly spicy odor of moderate to poor tenacity.

This cyclic terpene ketone has been made available mainly for the purpose of supplying the main component of Hyssop oil, which is relatively expensive and occasionally scarce on the market. It is a minor, but highly appreciated ingredient in certain topnote compositions for fine perfumes, and it is also used to a minor extent in flavor compositions for seasonings, etc.

Apart from this special application, there is no significant use for the subject material in perfumes or flavors.

Prod.:

1) from *alpha*-Pinene, via Nitrosopinene, reduced to the title material with Zinc dust or catalytic hydrogenation.
2) from Verbanone – also obtained by synthetic way.
3) from Pinonic acid ethyl ether.
4) by isolation from Hyssop oil (40-45% of the oil).

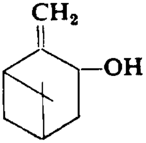
65-442; 67-567; 89-285; 163-65; 163-234; 163-373;

## 2623: PINOCARVEOL

*cis-* and *trans-*, *dextro-* and *laevo*-forms are known.

The *trans-laevo*-isomer is the naturally occurring form.

The *cis-dextro*-isomer is the most common synthetic form.



$C_{10}H_{16}O = 152.24$

Viscous, slightly yellowish or pale straw-colored oil. Sp.Gr. 0.98.

B.P. 210° C. M.P. 5° C. (*trans-*).

B.P. 217° C. M.P. 51° C. (*cis-*).

Insoluble in water, soluble in alcohol and oils.

Warm-woody-balsamic, slightly piney-fennel-like odor of moderate to poor tenacity. Progressive polymerization and/or oxidation during storage of this material increases the viscosity and changes the odor to a weaker, but more piney-resinous odor.

This cyclic terpene alcohol has been used occasionally in perfume compositions since at times the material has been commercially available as an intermediate. However, it is not regularly available and such interruptions in supply are usually enough to kill any further interest in a material if it is not highly interesting in the first place.

Briefly, the title material is not urgently needed by the perfume industry.

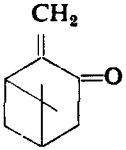
Prod.:

1) from Pinyl aminoacetate or -nitrate with Nitrous acid.
2) by isolation from Eucalyptus oil tail fractions.
3) by Meerwein-Ponndorf-Verley reduction of Pinocarvone.
4) by Autoxidation of *beta*-Pinene with Cobalt siccative or by oxidation with Selenium oxide.

65-231; 67-572; 88-213; 163-65; 163-373;

## 2624: PINOCARVONE

The naturally occurring material is *laevo*-Pinocarvone.



$C_{10}H_{14}O = 150.22$

Pale yellowish or straw-colored liquid. Insoluble in water, soluble in alcohol and oils.

Decomposes easily under exposure to air and/or moisture, Carvone being one of the degradation products. Very sensitive to acid.

Powerful camphoraceous-minty odor of moderate to poor stability, but good diffusive power. The fact that the material is stable under mildly alkaline conditions has contributed to the apparent interest in the subject material. In spite of its many serious drawbacks, it has attracted some attention in perfumery research, and it has been available as a by-product from the rectification of Spanish Eucalyptus oil at a very low price.

On the other hand, the volume needed of any interesting material for perfuming of household products, soaps, detergents, etc. is so enormous, that this fact alone creates a problem for any direct or indirect derivative of a natural product.

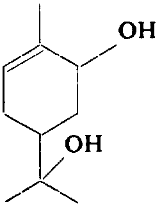
The material is briefly mentioned in this work because of the temporary interest it has created, and also in order to complete the description of the cyclic terpene ketone series.

Prod.:
1) by isolation from the tail fractions of Spanish Eucalyptus oil. These fractions contain about 15% total ketones.
2) by hydrolysis of Nitrosopinene with Oxalic acid.

65-446; 67-572; 89-349; 163-65; 163-234;

## 2625: PINOL HYDRATE

Sobrerol.
Sobrerene dihydrate.
*iso-1-para*-Menthene-*6,8*-diol.



$C_{10}H_{18}O_2 = 170.25$

White or colorless crystals. M.P. 148° C.

Insoluble in water, soluble in alcohol and oils.

Powerful camphoraceous odor, diffusive and warm, of poor tenacity.

This material is briefly mentioned because it has a certain potential as a fragrance chemical, and it can be produced at a very low cost. It is also closely related to Pinol, which is formed in the production of Pinene nitrosochloride, an intermediate in the manufacture of Pinocarvone (see that monograph).

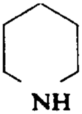
The author is not aware of any extensive use of the title material in perfumes or flavors, but it could find use in detergent perfumes, fragrances for household products, etc.

Prod.: by hydrolytic autoxidation of *alpha*-Pinene. It is also formed by heating of Pinol (see above), or by treatment of Pinene with Lead tetra-acetate.

65-58; 65-713; 67-539; 88-128; 160-1172; 163-65; 163-234;

## 2626: PIPERIDINE

Hexahydro pyridine.
Pentamethylenimine.
Hexazane.



$C_5H_{11}N = 85.15$

Colorless oily liquid. Acquires pale amber color upon storage if exposed to air and daylight. Sp.Gr. 0.86. B.P. 106° C.

Miscible with water, soluble in alcohol and oils.

The material forms a solid hydrochloride, soluble in water and alcohol.

Heavy-sweet, nauseating, floral-animal odor of great diffusive power and poor tenacity.

This material is used in small amounts in perfume compositions. Its effect on exotic floral fragrance bases is quite interesting, and unquestionably attractive, since the "trick" has success to prove it. However, one may prefer to think twice before this material is used in any new composition. It is true that the standard excuse for the use of potentially hazardous materials in food and cosmetics is the "extreme dilution in the functional product". The problem is just that no one has set the threshold yet. Exactly what is the "hazardous level" of such material?

A concentration of 10 to 20 ppm is not abnormal in a functional product, since the title material may enter a fragrance composition at the rate of 0.1 to 0.5%. A perfume base (intended for further composition work) may contain as much as 1 to 1.5% of the title material.

But this is not all. The material is permitted for use in food flavors and the use in spice blends may bring a final concentration in the functional product up to 0.1 to 5 ppm. If we decide to compare this against Nitrobenzene (which is *not* permitted), literature sources indicate that Piperidine is considered 1½ times as toxic as Nitrobenzene!

It is sometimes hard to understand for anyone who is not a toxicologist or pharmacologist, but it would be comforting to know what the experts consider "hazardous level" before we indulge in further use of this and similar materials. After all, they are not indispensable in perfumes or in flavors. The mere fact that Piperidine is related to one of the pungent principles in Black Pepper does not mean that it is absolutely necessary.

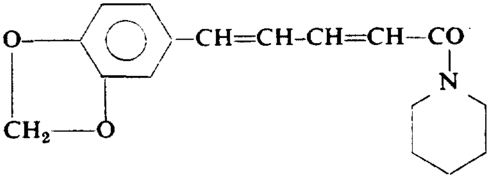
G.R.A.S. F.E.M.A. No.2908.

Prod.: from Pyridine by electrolytic reduction.

26-660; 69-570; 90-810; 100-822; 140-175; 160-1172; B-XX-6;

## 2627: PIPERINE

*l*-Piperoyl piperidine.



$C_{17}H_{19}NO_3 = 285.35$

White crystals. M.P. 130° C. Sp.Gr. 1.19 (liquid).

Slightly soluble in water, 10% soluble in alcohol, soluble only in certain oils.

Virtually odorless when pure. No initial taste, but very soon after application to the oral mucous membranes a hot, burning mouthfeel occurs in the back of the mouth and near the throat.

This material is one of the pungent principles in Black Pepper. It is accompanied by its isomer, Chavicine (see monograph) which is much more pungent, but not nearly as stable as Piperine. This fact may account for the loss of pungency upon ageing of Pepper.

This material is (obviously) not used in fragrances.

It finds use in flavor compositions, not only as ingredient in artificial Black Pepper, but also in various spice blends, and as an additive to the flavor composition used in "Celery Soda" (a carbonated beverage of sweet, but pungent Celery flavor, sometimes used as an appetizer).

Minute traces are also used in various types of Brandy to introduce a "hot" taste, actually it "sensitizes" the mouth and the flavor receptacles, indirectly.

The concentration in functional products is normally very low, about 0.01 ppm, except in special cases of needed pungency, e. g. Pickle flavors, etc.

The material is a powerful insecticide. Related derivatives of Heliotropine are used as insecticides and insecticide "boosters".

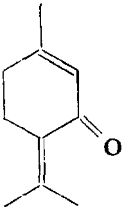
G.R.A.S. F.E.M.A. No.2909.

Prod.: from Piperonyl chloride and Piperidine.

26-732; 69-578; 100-823; 140-175; 158-213; 160-1174;

## 2628: PIPERITENONE

*para*-Mentha-*1*:*4*(*8*)-dien-*3*-one.
*1*-Methyl-*4*-*iso*-propylidene-*1*-cyclohexen-*3*-one.



$C_{10}H_{14}O = 150.22$

Pale yellowish or pale amber-colored oily liquid. B.P. 233° C. Sp.Gr. 0.98.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, sharp-minty, bitter-herbaceous odor of moderate tenacity.

If this material were available in quantity and at low cost, it would undoubtedly find very good use in perfume compositions for soaps, detergents, etc.

However, it has so far only appeared as a modest component of Pennyroyal oil (Moroccan), and its supply is therefore strictly limited.

It is briefly mentioned here among related materials as example of certain perfume materials which may become available if new chemical processes should happen to include these as intermediates or perhaps as end-products. It has some chemical interest in that it can be hydrogenated to Menthol.

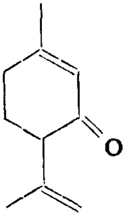
Prod.: from Moroccan Pennyroyal oil. The oil contains approximately 20% Piperitenone and 3% *iso*-Piperitenone, which inevitably accompanies the title material.

Piperitenone could be classified as moderately toxic. 10 grams present a hazard to an adult human being.

65-416; 67-529; 89-247; 163-234; 163-373;

## 2629: iso-PIPERITENONE

*para*-Mentha-*1*,*8*(*9*)-dien-*3*-one.
*1*-Methyl-*4*-*iso*-propenyl-*1*-cyclohexen-*3*-one.



$C_{10}H_{14}O = 150.22$

Pale yellowish oily liquid. B.P. 226° C. Sp.Gr. 0.97.

Practically insoluble in water, soluble in alcohol and oils.

The comments made on Piperitenone (see previous monograph) could be repeated here. Only this ketone is even more scarce and difficult to isolate. It would have potential as a perfume material if new chemical syntheses produced this material at a reasonable price and in sizeable volume.

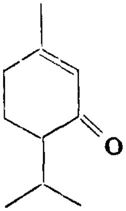
Its odor is powerful, diffusive, sweeter than that of the Piperitenone, but equally minty, penetrating and of moderate tenacity.

Prod.: see Piperitenone.

67-529; 89-247; 163-373;

## 2630: PIPERITONE

*1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*3*-one.
*para*-Menth-*1*-en-*3*-one.
The commercial material is mostly *laevo*-Piperitone.



$C_{10}H_{16}O = 152.24$

Colorless liquid. Sp.Gr. 0.93. B.P. 233° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, fresh-minty-camphoraceous odor. The material may turn darker yellow and its odor become more tobacco-herbaceous upon ageing.

This material has found some use in perfume compositions, mainly in masking odors for industrial purposes, inexpensive room-fresheners, etc. In certain industrial areas, however, enourmous amounts of "terpene fractions" from various perfume chemical processes are available at very low cost, and they are widely used for masking purposes. Competition has thus brought down the cost of perfume raw materials for masking purposes to a level where "pure" materials can hardly enter at all.

The cyclic ketone is more commonly used in flavor compositions, particularly in spice complexes with Caraway, Estragon, etc., and in fruit complexes, mint flavors, etc. Now and then it becomes "fashionable" in dentifrice preparations where larger amounts are used.

The concentration normally used is equivalent to about 1 to 20 ppm in the finished product.

The title ketone is also used in the manufacture of Menthol and Thymol.

G.R.A.S. F.E.M.A. No.2910.

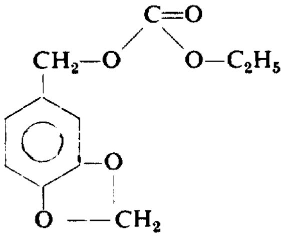
Prod.:

1) by isolation from Japanese Mint oil (*dextro*-Piperitone).
2) by isolation from Eucalyptus dives oil (*laevo*-Piperitone).
3) by hydrogenation of Diosphenol. (1069).
4) by reduction of *5*-Methyl-*2*-*iso*-propylanisole with Sodium in liquid Ammonia.
5) *laevo*-Piperitone can also be produced from *laevo-beta*-Pinene via *l*-Limonene, by hydrogenation to *l*-Carvomenthene, and via 4 further intermediate steps to the title material.

7-175; 67-525; 89-213; 100-823; 140-167; 65-396; 163-65; 163-234; 163-373; 104-229; Glidden (1966);

## 2631: PIPERONYL ETHYLCARBONATE

Heliotropyl ethylcarbonate.



$C_{11}H_{12}O_5 = 224.22$

Colorless viscous liquid, solidifying in the cold.

Practically insoluble in water, soluble in alcohol and oils.

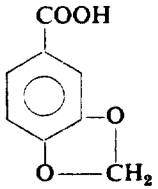
Very delicate, sweet-powdery, musky-floral odor of excellent tenacity.

This material has found some use in perfume formulation. It is rarely offered under its proper chemical name, but it enters various specialties and bases in a relatively high percentage. Its delicate, floral note and outstanding tenacity are used in modern creations, mainly in combination with high-grade Methylionones, macrocyclic musks, new Ambregris materials, refined Vetiver products, etc.

Prod.: from Piperonyl alcohol and Ethylalcohol with Phosgene.

## 2632: PIPERONYLIC ACID

Piperonilic acid.
Heliotropic acid.
*3,4*-Methylene dioxybenzoic acid.



$C_8H_6O_4 = 166.14$

White crystals. M.P. 230° C.

Slightly soluble in water, soluble in hot water. Poorly soluble in cold alcohol, soluble in hot alcohol. Soluble in certain oils, insoluble in most other oils.

The methyl ester is a white crystalline material M.P. 53° C.

Piperonylic acid has a faint, but very tenacious, sweet-balsamic odor with a discretely animal undertone.

The idea, that the aldehyde group is the main offender in the Heliotropine molecule has probably tempted perfume chemists to suggest the title material. It has relatively little perfumery value, but it does have a perceptible fixative value, and it will not cause the same type of incompatibility trouble as encountered with Heliotropine (Amines, Schiff's bases, etc.).

The methylester is mentioned above because it has some odor value (see monograph), but there is reason to believe that the salts of Piperonylic acid are odorless. Under mildly alkaline conditions (soap, etc.) one can therefore assume that the title material has no odor value.

The acid finds some use in face powder and cream perfumes, where tenacity and lasting powdery sweetness are often desirable.

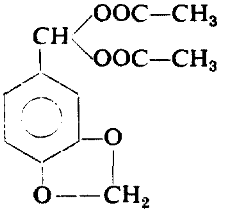
Prod.:

1) by oxidation of Heliotropine with Potassium permanganate.
2) also by direct oxidation from Safrole.

72-88; 68-775; 90-555; 100-824; 26-660; B-XIX-269;

## 2633: PIPERONYLIDENE DIACETATE

Heliotropylidene diacetate.



$C_{12}H_{12}O_6 = 252.23$

White crystals.

Insoluble in water, soluble in alcohol and oils.

Delicate, yet relatively powerful floral odor of excellent tenacity.

The title material, which appeared as a German patent many years ago, has been used in perfume compositions as a modifier for Heliotropine and Vanillin, briefly as a sweetener with floral character.

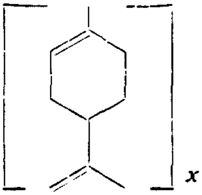
During the first few decades of the use of Heliotropine in perfumery, much attention was paid to the discoloration problem, which was generally attributed to the aldehyde group. By neutralizing this group, the problem should be reduced or solved, one thought.

However, none of the "non-aldehydic" Heliotropine derivatives have the power of Heliotropine itself, and many of the derivatives carry other hazards, such as slow decomposition resulting in off-odor, etc. The title material may produce acetic off-odor under storage and compound conditions, but it is otherwise quite interesting.

163-65; 163-373; (B.A.S.F. patent).

## 2634: POLYLIMONENE

A product consisting of polymerized Limonene with a structure of approximately:



($x = 2$ or 3).

Pale yellowish, viscous liquid.

Insoluble in water, poorly soluble in cold alcohol, soluble in hot alcohol and oils.

Very faint, sweet-balsamic-fruity odor of excellent tenacity. The odor varies according to origin and age of material.

The title material is used as a fixative in flavor compositions, mostly in fruit flavors intended for hard candy, etc., where stability against heat is important during the processing of the functional product.

The concentration used is relatively high, and may reach 5000 ppm in certain types of candy. At this level, the material does have a slightly pungent mouthfeel or taste, and should be accompanied by suitable sweetening and flavor-softening agents.

Prod.: by polymerization of Limonene, mostly from *dextro*-Limonene (or "Orange terpenes").

Approved for food use by F.E.M.A.

## 2635: POLYSORBATE

Under this title the following materials are briefly mentioned:

1) Polyoxyethylene (20) Sorbitan Monolaurate, known as Polysorbate 20.
2) Polyoxyethylene (20) Sorbitan Tristearate, known as Polysorbate 65.
3) Polyoxyethylene (20) Sorbitan Monostearate, known as Polysorbate 60.
4) Polyoxyethylene (20) Sorbitan Monooleate, known as Polysorbate 80.

The above materials represent the only materials of this type approved for use in food in the U.S.A.

They are sold under various trade names, but their chemical compositions are well known and clearly indicated.

The materials are viscous or very viscous pale yellowish or pale amber-colored liquids, with Specific gravity between 1.02 and 1.10, soluble in water, alcohol, Propylene glycol, vegetable oils, most flavor oils, but not in mineral oil.

They are used as emulsifiers in food, or as solubilizers in flavor compositions. It is common practice, when a flavor must be made miscible with water, to add Polysorbate under stirring to the flavor oil, normally in the amount of 2 to 4 parts of Polysorbate to one part of flavor oil (unless the flavor oil contains very large amounts of Propylene glycol). Water can then be added to the mixture slowly under stirring, producing an optically clear "solution".

The manufacturers of the title materials recognize that although the flavor industry is a small customer compared to the textile, paper- and other Polysorbate customers, the Polysorbates for flavor purpose must be particularly free from malodor. Special grades are usually available for food and flavors.

The subject materials produce almost neutral solutions in water, the pH of aqueous solutions being less than 7 but higher than 5.

The Polysorbates are manufactured from partial esters of the fatty acids with Sorbitol anhydride (Sorbitan) and related Hexitans. These esters are known as "Span"s, and their derivatives with Polyoxyethylene chains are known as "Tween"s, the subject materials. The Span products are generally oil-soluble, while the Tween products are generally water-soluble. They all have only very faint, warm-oily odor or practically no odor, while they do have a bitter taste in concentrations exceeding 500 ppm.

The American Food and Drug Administration has issued meticulously specified limitations for use of these materials in food. They are classified as "food additives", not as flavor materials.

Concentrations may vary from 100 to 1600 in various finished products, highest in baked goods. Exceptionally high concentrations are found in soups (up to 4000 ppm) and in dessert toppings (up to 12000 ppm). As an example, the limit is 4600 ppm (of Polysorbate 60 alone) in a cake icing or a cake filling, or 10000 ppm of the total combination of two or more of the emulsifiers.

100-833; 100-970; 162-695; (several suppliers issue detailed data and information).

## 2636: POTASSIUM ACETATE

$CH_3{-}COO{-}K$

$C_2H_3KO_2 = 98.15$

Colorless crystals, hygroscopic and deliquescent. M.P. 292° C.

65% soluble in water, 35% soluble in alcohol, insoluble in most oils.

Odorless when pure. The aqueous solution has an alkaline taste.

This salt is not classified as a flavor material, but as a food additive. Although it is beyond the scope of this work to discuss all food chemicals (i. e. "Chemicals in Food"), the author has preferred to include a few of the more common food additive chemicals.

The title material is occasionally used in carbonated beverages, mainly the type known in the U.S.A. as "Club Soda", in other countries called "Mineral water" or "White Soda" etc. The concentration is about 1 to 2 ppm and it serves several purposes, including that og being a buffer for the carbonation system.

G.R.A.S. F.E.M.A. No.2920.

26-288; 100-836;

## 2637: POTASSIUM BICARBONATE

Potassium acid carbonate.

$KHCO_3 = 100.12$

Colorless, transparent prismatic crystals or white granular powder. Decomposes when heated, liberating Water and Carbon dioxide, and leaving Potassium carbonate behind. This is the effect utilized in baking powder.

Odorless when pure. The material or its aqueous solution have a flat, mildly alkaline taste.

26% soluble in water, almost insoluble in alcohol and oils.

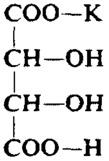
This material, sometimes known as "baking powder" (in which it is often a component) is used commonly in baking powders (for the above effect of liberating $CO_2$-gas) and in effervescent salts to assist in controlling the rate of effervescence.

G.R.A.S. (approved as a general purpose food additive).

26-288; 100-837;

## 2638: POTASSIUM BITARTRATE

Potassium acid tartrate.
Potassium hydrogen tartrate.
Cream of tartar.
Cremor tartari.



$$\begin{array}{l} COO{-}K \\ | \\ CH{-}OH \\ | \\ CH{-}OH \\ | \\ COO{-}H \end{array}$$

$C_4H_5KO_6 = 188.18$

Colorless or slightly opaque crystals or white crystalline powder. 0.6% soluble in water, 6% soluble in boiling water, almost insoluble in alcohol and oils.

Pleasant acid taste in aqueous solution. The dry material is odorless.

This material is used in baking powders, usually in combination with the Bicarbonate or one of the Ammonium carbonates.

It is classified as a general purpose food additive, and as such listed in the American G.R.A.S. list.

Prod.: The material appears in enormous quantities as a by-product in wine-making. It is extracted from the sediment of the fermentation vats.

26-294; 100-838;

## 2639: POTASSIUM SORBATE

Potassium-*2,4*-hexadienoate.

$CH_3—CH=CH—CH=CH—COO—K$

$C_6H_7KO_2 = 150.22$

Colorless crystals. Decompose at 270° C. before melting.

58% soluble in water, 7% soluble in alcohol at room temperature. Insoluble or poorly soluble in oils.

Odorless, but has a bland-acidulous taste in dilute aqueous solution.

Sorbic acid is a mold- and yeast-growth inhibitor, but it is poorly soluble in water. The Potassium salt has therefore been suggested for use in food products.

The concentration of this salt in the finished product will be about 100 to 1000 ppm, since the effective concentration of the salt is 0.01 to 0.1% in suitable combination with traces of other inhibitors. It is also customary to use traces of the acid along with the salt. In candy and other emulsified or non-homogeneous food products, it is of course possible to use the acid to a fuller extent, but the salt solution gives a safer distribution of the inhibitor.

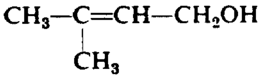
G.R.A.S. F.E.M.A. No.2921.

Classified as a chemical preservative.

100-846;

## 2640: PRENOL

*2*-Methylbuten-*2*-ol-*4*.
A hemiterpene alcohol.



$$\underset{\displaystyle CH_3}{CH_3—C}=CH—CH_2OH$$

(probable structure)

$C_5H_{10}O = 86.14$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, herbaceous-fruity-green, somewhat Lavender-like odor of poor tenacity.

The taste is – in high dilution – winey, Brandy-like, slightly green-fruity. The title alcohol is occasionally used as a trace component in imitation Raspberry flavor.

This alcohol, although it has been known for several decades, has only recently been made commercially available. Its present cost, however, is still rather prohibitive for a more extended use of this material, and it can only be used sparingly in Lavender because of the high cost of this alcohol.

It is nevertheless interesting, and its odor is quite characteristic and lively, inviting to further experimenting.

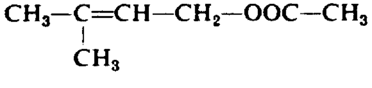
Prod.:

1) from Isoprene by hydration via Phenylacetate (see next monograph).
2) from Dimethyl vinylcarbinol with diluted Sulfuric acid.

10-30; 89-91;
(material from Compagnie Parento, Inc.).

## 2641: PRENYL ACETATE

*2*-Methylbuten-*2*-ol-4-acetate.



$$\underset{\displaystyle CH_3}{CH_3—C}=CH—CH_2—OOC—CH_3$$

$C_7H_{12}O_2 = 128.17$

Colorless mobile liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Fresh and very diffusive, fruity, Banana-like and Bergamot-like odor of poor tenacity.

Powerful, fruity and sweet, Pear-Banana-like taste at 10 ppm or lower. This material was made commercially available in 1966 at a time when Lavandin oil was scarce and expensive. Any material that could help improve an artificial Lavandin or Lavender was of immediate interest.

However, this material has found uses far beyond Lavandin, Lavender and Bergamot. In flavor compositions, for instance, its high cost is compensated for by its outstanding power. As a modifier for the Amylesters, it has great potential and is very interesting, but as a sweetening herbaceous ester, it is still far too expensive (about 15 times the cost of Linalyl acetate).

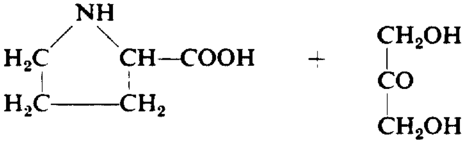
If increased use result in volume production, one may justly assume that this material can be produced at a much more attractive price and thus come into entirely new fields of perfumery application.

Prod.: by catalytic hydration of Isoprene in glacial Acetic acid.

10-30; 89-91;
(material from Compagnie Parento, Inc.).

## 2642: PROLIN-DIHYDROXYACETONE

Proline-dihydroxyacetone.
An ill-defined product resulting from a reaction between Prolin and Dihydroxyacetone:



The reaction mixture has a pronounced odor of freshly baked bread, and is used in flavor creation as such – for reconstitution of the desirable odor in bread, and for "bake-shop-odor" sprays, used in super-markets to psychologically attract customers to the bread section and to give the customers the impression that "baking is done on the premises".

Prolamins are found in Cereal seeds. They contain Proline and Glutamine residues, and the above process actually reproduces the natural process in which the bread flavor (or part of it) is developed.

Proline is listed as G.R.A.S., classified as a nutrient or a dietary supplement.

100-856; 66-1332;
see also: Dihydroxyacetone.

## 2643: PROPARGYL ALCOHOL

*2*-Propyl-*1*-ol.
Ethynyl carbinol.
Acetylene carbinol.
Propiolic alcohol.

$CH\equiv C-CH_2OH$

$C_3H_4O = 56.06$

Colorless mobile liquid. Sp.Gr. 0.97.
B.P. 114° C.

Miscible with water, alcohol and oils, but not soluble in mineral oil, many hydrocarbons, etc.

The material tends to polymerize if exposed to heat or in contact with alkali.

Powerful and very diffusive, but rather pleasant, foliage-green, Geranium-leaf-like odor of poor tenacity. Gassy at high concentrations, but pleasant-sweet in extreme dilution.

The title material is considered a hazard to human skin. The vapors have a depressing effect upon the human CNS.

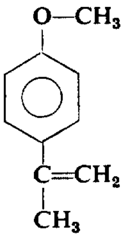
This alcohol is briefly mentioned because it is often included in perfume chemical literature, and one could have the impression that the material is useful and harmless for such purpose. It has been suggested as a "Geranium-green" fragrance chemical, but the author finds that we are very well stocked up with safer and better fragrance chemicals of that odor type.

1) as a by-product in the manufacture of *2*-Butyne-*1,4*-diol from Acetylene plus Formaldehyde in presence of a catalyst.
2) from *beta*-Chloroallylalcohol plus Sodium hydroxide.

26-662; 31-16; 66-318; 100-859; 160-1192; B-1-454;

## 2644: para-iso-**PROPENYL ANISOLE**

*4-iso*-Propenyl-*1*-methoxybenzene.
*1*-Methoxy-*4-iso*-propenylbenzene.



$C_{10}H_{12}O$ = 148.21

Colorless or opaque-whitish crystalline mass. M.P. 33° C. The liquid is almost colorless. B.P. 222° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, warm pungent, anisic-caraway-like odor of moderate to poor tenacity.

The title Phenolether, which is an isomer of Anethole and Estragole, has been suggested for use in perfume compositions.

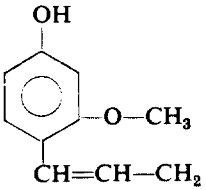
It seems, however, that the material has failed to arouse any enthousiasm among perfumers or flavorists. Its odor type does not allow for a very high cost, since many materials of similar odor type are available at very low cost. And this may be the fact that put the title material out of the perfume laboratory. It is simply too expensive for its odor type.

Prod.: from *para*-Anisole carboxylic ester and Methyl magnesium iodide.

31-150; 68-971;

## 2645: **PROPENYL**-meta-**CRESOL METHYLETHER**

*para*-Propenyl-*meta*-methoxyphenol.
Methoxy hydroxy propenyl benzene.
An isomer of *iso*-Eugenol.
A lower homologue of Vanitrope (see next monograph).



$C_{10}H_{12}O_2$ = 164.21

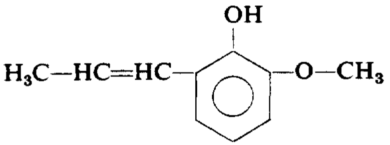
White crystals.

Almost insoluble in water, soluble in alcohol and oils.

Warm, sweet, but slightly "smokey" odor of good tenacity. Sweet, Vanilla-like taste in extreme dilution, but "medicinal-phenolic" at concentrations above 10 ppm.

The title material has come out of Vanillin research, and it was one of rather few chemicals being considered at all. However, its medicinal off-odor and flavor seem to be serious disadvantages, and blending with Vanillin or "Ethylvanillin" does not seem to solve the problem (such as it has been partly solved in the use of Vanitrope).

There is considerable chance of confusing this item with *ortho-iso*-Eugenol, which is *6*-Propenyl guaiacol, or:
*1*-Hydroxy-*2*-methoxy-*6*-propenylbenzene:



$C_{10}H_{12}O_2$ = 164.21

White crystals, M.P. 78° C. Faint, sweet-balsamic odor of excellent tenacity. Produced from *ortho*-Eugenol by isomerization with Sodium hydroxide.

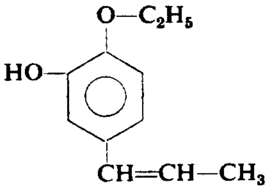
The author is inclined to believe that perfumery literature often refers to this item, when the title name is mentioned.

None of the two materials have achieved any importance in perfume or flavor creation.

68-976;

# 2646: PROPENYL GUAETHOL

"Vanitrope" (Shulton, Inc.).
Methyl-*iso*-chavibetol.
*1*-Ethoxy-*2*-hydroxy-*4*-propenylbenzene.
*6*-Ethoxy-*meta*-anol.
Hydroxymethyl anethole.
*5*-Propenyl-*2*-ethoxyphenol.



$C_{11}H_{14}O_2 = 178.23$

White or colorless crystalline powder.

M.P. 86° C. Sublimes when heated under vacuum.

10% soluble in alcohol, 4% soluble in Propylene glycol, 4% soluble in Polysorbate 80, 20% soluble in Benzylalcohol, slightly soluble in water, soluble in most perfume and flavor oils.

Intensely sweet, but in the dry state rather medicinal-phenolic odor, often described as "drug store odor". The sweet odor is more perceptible at high dilution, while the phenolic odor seems to vanish at such low concentrations.

Below 5 ppm, the taste is sweet, Vanilla-like, warm-spicy, pleasant, but at higher levels the phenolic-medicinal taste appears and may dominate the flavor picture. The minimum perceptible is below 1 ppm.

This Guaiacol-derivative of the Vanillin family is one of the most successful members of that group since the appearance of "Ethylvanillin". When used in conjunction with Vanillin and "Ethylvanillin", the title material is capable of supplying an enormous Vanilla-like power to the flavor composition. The manufacturer originally estimated the power at 25 times that of Vanillin, while in actual use one may calculate about 15-16 times the Vanillin power. There is a limit to how much Vanitrope can be used in a composition, and the upper limit is normally about 4 to 5% by weight of the Vanillin or "Ethylvanillin" used in conjunction with the title material.

In other words, the "Vanilla" flavor of the composition can be approximately doubled in strength if the composition is Vanillin plus Vanitrope. "Ethylvanillin" (see monograph Ethylvanillin, commercial name) is approximately 2½ times stronger than Vanillin, and it is therefore possible to make a powder-mixture of 3½ to 4 times the Vanillin-flavor power from Vanitrope plus "Ethylvanillin".

Vanitrope costs about 4 times as much as "Ethylvanillin" and 9 or 10 times as much as Vanillin. The savings in using Vanitrope are very small, but the advantage is in the added, Vanilla-like character of the flavor. Furthermore, certain flavor chemicals seem to have synergistic effect upon the Vanilla flavor of the title material (Heliotropine, Creosol, Palatone, etc.).

The title material is used in many types of flavor composition: Chocolate, Maple, Nut, Vanilla, Butterscotch, Rum, Caramel, etc. and it may be used exclusively as a sweetener at very low concentration, or as a Vanilla-flavor at higher levels. The normal concentration in finished products is 2 to 25 ppm.

G.R.A.S. F.E.M.A. No.2922.

The toxicity of this material has been estimated as equal to that of Vanillin, gram for gram. In other words, it is less toxic as a Vanillin replacement.

The title material is occasionally used in perfumes as a sweetener or as a replacement for Vanillin, if there is a discoloration problem involved. By using less Vanitrope to achieve the same Vanilla-sweetness, the perfumer can reduce the amount of sensitive Aldehyde-group per weight unit of the perfume, and thus reduce the risk of discoloration in the ratio equivalent to the Vanillin/Vanitrope substitution. It is characteristic of Vanillin-discoloration that it appears at a certain level of Vanillin concentration, and not at all below that level.

A reduction of the percentage of the trouble-making aldehyde group will therefore often solve the problem.

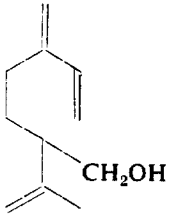
Vanitrope suffers from the same drawbacks as Vanillin: it is sensitive to alkali, iron and direct sunlight. It produces dark adducts with Anthranilates, Quinolines and Indoles.

Prod.: from Eugenol ethylether by heating in ethylalcoholic alkaline solution.

53-373; 88-1/7; 100-860; 156-379; 163-235; 163-243;
see also: Ethyl-*iso*-eugenol (1223), and
*5*-Propyl-*2*-ethoxyphenol (2704).

## 2647: 2-iso-**PROPENYL**-5-**METHYLENE**-6-**HEPTEN**-1-**OL**

"Methyl-*iso*-geraniol".
*2,6,7*-Trimethylene-*3*-hydroxymethylheptane.



$C_{11}H_{18}O = 166.27$

Colorless or pale straw-colored oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-rosy, slightly waxy odor of moderate tenacity. Overall fresher than Geraniol, and much stronger. The material tends to polymerize upon standing, and it is not very stable in soap.

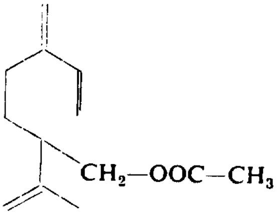
This alcohol, only rarely offered commercially, and normally under trade name only, has been suggested for use in perfume compositions as a powerful ingredient for floral, particularly rosy, fragrance types. Its acetate is more stable, fresher smelling and more versatile in use (see next monograph).

In view of the fact that the title material has been known for quite a number of years and not reached any level of fame, it could be reasonably safe to say that it is of little interest to the perfumer, and it may soon become obsolete.

163-360;

## 2648: 2-iso-**PROPENYL**-5-**METHYLENE**-6-**HEPTEN**-1-**YL ACETATE**

"Methyl-*iso*-geranyl acetate".



$C_{13}H_{20}O_2 = 208.30$

Colorless or very pale straw-colored mobile liquid.

Insoluble in water, soluble in alcohol and oils.

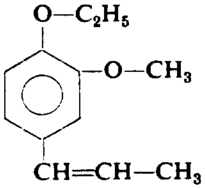
Fresh, leafy-rosy, delicately green, almost vegetable-green odor of pleasant, yet powerful sweetness of Geranium type. Moderate tenacity.

This ester has been suggested for use in soap perfumes because of its great odor volume and refreshing fragrance type, applicable to floral as well as citrusy, particularly Lemon-Bergamot types of soap and cosmetic perfumes. It supports Geranium oil in freshness, gives power to the Citrus oils, and introduces light notes in Lavender or Clary Sage or Fougères. It blends excellently with Oakmoss products.

Prod.: by Acetylation of Methyl-*iso*-geraniol (see previous monograph).

## 2649: PROPENYL METHYL GUAETHOL

"Methylvanitrope".
"Homovanitrope".
*para*-Propenylcatechol ethyl methyl ether.
"Methyl ethyl-*iso*-eugenol".



$C_{12}H_{16}O_2 = 192.26$

White or colorless crystals.

Practically insoluble in water, soluble in alcohol and oils.

Caramellic-sweet, very tenacious, warm and deep-spicy odor.

Intensely sweet, remotely Vanilla-like, caramellic-spicy taste in concentrations below 5 ppm.

This material, rarely available under its proper chemical name, has been suggested for use in perfumes. It is not listed in the American G.R.A.S. list, but it could undoubtedly find use in flavor compositions outside of the U.S.A.

It is an excellent sweetener, stable in soap and it does not discolor in cosmetic preparations as easily as Eugenol, Vanillin, etc. However, the cosmetic skin research is very concerned about the Propenyl group and that group is accused of being a hazard to the human skin, a fact which would bring Eugenolderivatives under the limelight and possibly ban them from use in cosmetic fragrances.

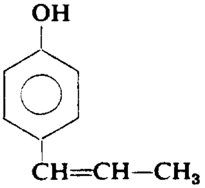
But until more solid proof of such hazards have been published and authoritatively treated, the perfumers will use these materials, many of which have absolutely no substitute.

The title material may meanwhile become a popular fragrance chemical for its very pleasant effect and great tenacity. It blends very well with Oakmoss, Ylang, Methylionones, Patchouli, Coumarins, etc.

Prod.: from Propenyl guaethol by Methylation. See monograph on Propenyl guaethol (Vanitrope).

## 2650: PROPENYL PHENOL

*para*-Anol.
*1*¹-Propenylphenol.
*iso*-Chavicol.
*4*-Hydroxy-*1*-para-propenylbenzene.
Paranol.



$C_9H_{10}O = 134.18$

Colorless leaflets. M.P. 94° C. B.P. 250° C. (decomposes).

Poorly soluble in cold water, slightly soluble in hot water, soluble in alcohol and oils.

Mild, warm-spicy, moderately tenacious odor resembling the odor of dry leaves (or, more romantically, odor of "feuilles mortes"), with the discretely phenolic, tealike odor, sometimes encountered in Chinese tea.

Spicy taste and warm or burning mouthfeel at concentrations above 40 ppm.

This phenol is used in perfume compositions where the presence of a phenol is compatible. The title material will discolor under alkaline conditions and in presence of iron. Its low cost makes it elegible for perfumes and masking odors for industrial purposes, but it is also interesting to use the material in better perfumes, e. g. in combination with Oakmoss, with which it makes very attractive blends. Supported by Methyleugenol and Vetiver, it can form part of novel fixative undertone bases, etc.

Prod.:

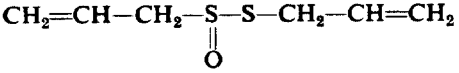
1) by isomerization of Anethole by heating with Potassium hydroxide.

2) by heating of Chavicol with Potassium hydroxide.
3) from *para*-Hydroxybenzaldehyde and Ethylmagnesium iodide.

31-38; 68-969; 90-490; 100-84; 160-808; 163-7; 163-176;

## 2651: 2-PROPENYL-2-PROPENE THIOSULFINATE

Allicin.



$$CH_2{=}CH{-}CH_2{-}\underset{\substack{\|\\ O}}{S}{-}S{-}CH_2{-}CH{=}CH_2$$

$C_6H_{10}OS_2 = 162.28$

Yellowish mobile oil.

Almost insoluble in water, soluble in alcohol and oils.

Extremely powerful and penetrating odor of fresh Garlic.

The title material is considered to be the most important flavor component of the volatile oil from fresh Garlic.

It constitutes approximately 0.15% by weight of the fresh plant material.

Since the title material has been synthesized, it has found use in food flavoring to reconstitute the flavor in dried or processed Garlic, in meats, sausages, dressings, spice blends, etc.

The chemical is not specifically listed in the American G.R.A.S. list, while Garlic extract is included in that list.

The results from intensive research into the natural components of Garlic and Onion flavor is of comparatively recent date, and it is too early to make any definite statements as to the future importance of the title material.

Prod.: from Di-propenyl disulfide by oxidation, e. g. with Periodic acid.

157-391;

## 2652: PROPIONALDEHYDE

Propanal.
Methylacetaldehyde.
Propylaldehyde (outdated name).

$CH_3{-}CH_2{-}CHO$

$C_3H_6O = 58.08$

Colorless mobile liquid. B.P. 49° C.
Sp.Gr. 0.81.

20% soluble in water, miscible with Propylene glycol, Glycerin, alcohol and oils.

Very diffusive and penetrating, suffocating odor with choking effect upon the respiratory system. Very poor tenacity. In extreme dilution an odor of roasted Coffee appears.

Since the material is water-soluble, its flavor effect in aqueous media is not so enormous. Concentrations near 10 ppm have a sweet-ethereal, green-caramellic taste. Higher concentrations tend to give burning mouthfeel or pungent taste.

The title aldehyde is not used in perfume compositions, except for very rare cases of trace addition to special bases or artificial essential oils, flower absolutes, etc.

It is used in flavor compositions for its lifting-ethereal effect, which is particularly attractive in imitation Apple. The concentration in the finished product will be about 5 to 12 ppm.

Prod.: from Propylalcohol over Copper at high temperature, or by oxidation with Potassium bichromate/acid.

G.R.A.S. F.E.M.A. No.2923.

26-662; 31-36; 31-37; 66-477; 89-10; 100-860; 160-1186; 163-65; B-I-629;

## 2653: PROPIONE

*3*-Pentanone.
Diethyl ketone.
Ethylketone.
*symmetric*-Dimethylacetone.
Methacetone.

$CH_3—CH_2—CO—CH_2—CH_3$

$C_5H_{10}O = 86.14$

Colorless liquid. Sp.Gr. 0.82. B.P. 103° C.

5% soluble in water, soluble in Propylene glycol and Glycerin, miscible with alcohol and oils.

Pleasant, ethereal-warm, diffusive odor, milder than that of Acetone, but similar in character.

Occasionally used as part of a masking odor for industrial purposes, or as co-solvent in masking odor compositions where poorly soluble terpenes etc., are components.

Otherwise rarely used in perfumes and not used in flavor compositions.

Prod.:
1) from Propyl alcohol.
2) from Propionic acid.

26-500; 31-80; 66-517; 100-353; 160-1146; B-I-679;

## 2654: PROPIONIC ACID

Propanoic acid.
Ethylformic acid.
Methylacetic acid.

$CH_3—CH_2—COOH$

$C_3H_6O_2 = 74.08$

Colorless liquid. Sp.Gr. 0.99. B.P. 141° C.

Miscible with water, Propylene glycol, Glycerin, alcohol, oils, etc.

Pungent sour odor reminiscent of sour Milk, Cheese or sour Butter.

Sour taste in aqueous solution, pleasant-sour at concentrations below 100 ppm. Higher concentrations seem to produce the cheesey-sour, more unpleasant taste.

This material is probably not used in perfumes at all.

It is widely used in food products, and also in many flavor compositions. As a fungicide or fungistat, it is used at the concentration of 0.25% to 3.6% equivalent to 2500 to 36000 ppm in the finished product. However, the acid will disappear largely from most of these products prior to consumption, due to evaporation. In semi-finished bread, the acid will disappear in the final oven-treatment of the bread.

In fruit and Butter imitation flavors, in imitation Raspberry, Strawberry, Cognac, etc. the acid is used in smaller amounts, and the concentration in finished products with such flavors will be about 1 to 600 ppm, highest in Butter- and Cheese-flavored products.

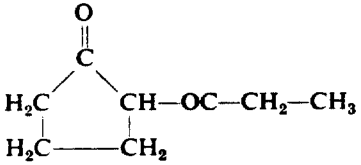
Propionic acid is manufactured on a very large scale and in an extremely high degree of purity.

Prod.:
1) from Ethylene with Carbon monoxide and steam.
2) from Ethyl alcohol with Carbon monoxide and a catalyst.
3) as a by-product from wood tar distillation.
4) by micro-organism activity on various materials.

G.R.A.S. F.E.M.A. No.2924.

26-662; 66-571; 90-58; 100-860; 160-1188; B-II-234;

## 2655: 2-PROPIONYL CYCLOPENTANONE



$C_8H_{12}O_2 = 140.18$

Colorless liquid. B.P. 200° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, semi-dry, but pleasant odor of haylike or cured tobacco-leaf-like character and moderate to poor tenacity.

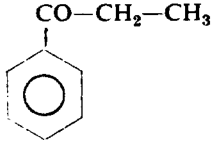
This ketone is rarely found in price lists, but it may be manufactured by the individual user or interested party. It may be a component of one or more successful perfume bases, and it is quite a versatile material. Its herbaceous character is of such Nature, that it is very suitable for Jasmin, Tuberose and other heavy floral bases, while it produces novel nuances with Methylionones or Vetiver products, Oakmoss, Amylsalicylate (excellent modification for Fougère), with Patchouli, the Eugenols, etc.

The material belongs to a chemical family yet far from fully exploited by the perfume chemists, and it would be interesting to see a further number of members of this family on the market.

Prod.: from Cyclopentanone with Propionyl chloride. A process based upon the intramolecular cyclization of alifatic ketone-carboxylic acids has also been suggested.

## 2656: PROPIOPHENONE

Ethyl phenyl ketone.
Phenyl ethyl ketone.
*1*-Phenyl-*1*-propanone.
Propionyl benzene.



$C_9H_{10}O = 134.18$

Colorless leafy crystals. M.P. 21° C. or colorless oily liquid. Sp.Gr. 1.01. B.P. 218° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, warm-floral, moderately pungent-herbaceous odor of rather poor tenacity.

This higher homologue of Acetophenone (see also monographs on Methylacetophenone and Ethyl acetophenone) has found some use in perfume compositions for its powerful, herbaceous-floral effect, and for an overall to that of Ethylbenzoate, and it can be used in discrete amounts in Lilac, higher proportions in Hawthorne, Wistaria, Fougère, etc. It blends well with Cananga, Amylsalicylate, Anisaldehyde, Lavandin oil, etc. and it is relatively inexpensive.

It has that feature in common with Acetophenone, that it may produce truly pleasant olfactory effect in the hands of a skilled and experienced artist-perfumer, while it too often comes out rather "loud" of a compound created with less skill. This fact is sometimes translated so that Acetophenone (and Propiophenone) are "difficult" perfume materials. The truly creative perfumer might just take this as one more challenge to obtain new effects, regardless of the Nature of the raw materials.

Prod.: (several methods) e. g. from Propionyl chloride and Benzene with anhydrous Aluminum chloride.

26-548; 68-532; 100-861; 160-1190; 163-65; [illegible];234;200.

the acid will disappear largely from most of
these products prior to consumption, due to

## 2657: n-PROPYL ACETATE

$CH_3—CH_2—CH_2—OOC—CH_3$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. Sp.Gr. 0.89.
B.P. 102° C.

2% soluble in water, miscible with Propylene glycol, Glycerin, alcohol and oils.

Diffusive and fresh, ethereal-fruity, Pear-like odor of poor tenacity.

Sweet Raspberry-Pear-like taste in concentrations near 20 ppm.

This ester is flammable and its vapors form explosive mixtures with air.

Propylacetate is rarely used in perfume compositions, except occasionally as part of topnotecompositions or additives to Citrus colognes, etc. to introduce ethereal lift and volatile "freshness" with the alcohol and the initial notes of the fragrance (when used in alcoholic solution).

The ester is widely used in flavor compositions as a major (by volume, not by flavor power) part of Strawberry, Raspberry, Blackcurrant, Apple, Pear, Cherry, Peach, Pineapple, Melon, Cucumber, Rum, etc. and in "Tutti-fruitti" type to support the "flavor burst" initially.

The concentration is normally given at 5 to 15 ppm in the finished product, but the author would believe that much higher concentrations are used in some of the above types. The effect at 5 ppm in a composition flavor is near negligible, and it is barely perceptible if no other flavor material is present. Concentrations up to 150 ppm would seem more practical.

The name "Propyl acetate" is often used to cover the *iso*-Propyl acetate, see next monograph.

G.R.A.S. F.E.M.A. No.2925.

Prod.: by azeotropic esterification of *n*-Propanol with Acetic acid.

26-662; 33-500; 33-621; 90-196; 100-862; 140-134; 160-772; 163-65; 163-235; B-II-129;

## 2658: iso-PROPYL ACETATE

Dimethyl carbinyl acetate.

$(CH_3)_2CH—OOC—CH_3$

$C_5H_{10}O_2 = 102.14$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 89° C.

3% soluble in water, miscible with Propylene glycol, Glycerin, alcohol and oils.

Very diffusive, fruity-ethereal odor of very poor tenacity.

Sweet Apple-like taste in concentrations near 40 ppm.

This ester is even more volatile than the *n*-Propyl acetate (see previous monograph) and it serves similar purposes. There is a slight difference in flavor, more than in odor. The title material is more Apple-like, less heavy-Raspberry-like in its taste.

It serves occasionally as a special "lift" to Citrus colognes and to the alcoholic odor of the alcoholic solution of Citrus perfumes and other light fragrances. Since the ester evaporates almost as fast as alcohol, it will "surround" the alcohol with a nuance of warmer, more ethereal, "aged" type of odor.

The chief application is, however, in flavor compositions. The title ester is used in imitation Apple, Pear, Blackcurrant, Peach, Rum, various fruit complexes and Liqueur flavors. Concentrations are about 20 to 80 ppm in the finished product. The author believes that concentrations are actually higher in many flavored products, but the figures given here are quoted from officially released information.

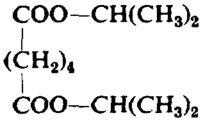
Prod.: by azeotropic esterification of *iso*-Propylalcohol with Acetic acid.

G.R.A.S. F.E.M.A. No.2926.

26-662; 33-500; 160-772; 163-210; 163-40; B-II-130;

## 2659: iso-PROPYL ADIPATE

Di-*iso*-propyl hexanedioate.
Di-*iso*-propyl-*1:4*-butanedicarboxylate.
Di-*iso*-propyl adipate.
Adipic acid, Di-*iso*-propylester.



$$\begin{array}{l} COO{-}CH(CH_3)_2 \\ | \\ (CH_2)_4 \\ | \\ COO{-}CH(CH_3)_2 \end{array}$$

$C_{12}H_{22}O_4 = 230.31$

Colorless oily liquid. Sp.Gr. 0.98.
B.P. 261° C.

Insoluble in water, miscible with alcohol and oils.

Practically odorless. The commercial product may have a faint "alcoholic" odor, barely perceptible in a container with the ester, but not on a perfume blotter.

This ester has been used as solvent for various perfume materials, such as resinoids, concretes, extracts, etc. to make them pourable and more handy for compounding purposes.

It has no odor value, but it will, if it is present in high proportion, have a depressing effect upon the overall odor of the composition. In case of use as an Oakmoss solvent/plasticizer, the material will only be present at the level of a few percent, and not influence the odor.

Although the perfumer has many solvents on hand for similar use, there are relatively few absolutely odorless, stable, soluble, high-boiling and inert solvents available, and the title material has the general prerequisites. It can not compete with Diethylphthalate *in* cost, but it is sometimes a better solvent for Oakmoss resinoid, etc.

Prod.: by azeotropic esterification of *iso*-Propanol with Adipic acid.

B-II-574; zweiter Ergänzungsband.

## 2660: n-PROPYL ALCOHOL

*1*-Propanol.
Ethylcarbinol.
Propylic alcohol.
Albacol.
Optal.

$CH_3{-}CH_2{-}CH_2OH$

$C_3H_8O = 60.10$

Colorless mobile liquid. Sp.Gr. 0.80.
B.P. 97° C.

Miscible with water, Propylene glycol, Glycerin, alcohol and oils.

Propylalcohol is flammable and its flashpoint is very near room temperature. Its vapors present therefore an explosion hazard.

The commercial product has an alcoholic-nauseating, sweet odor of very poor tenacity.

Highly purified Propyl alcohol has only a very faint odor, but it is apparently impractical to undertake such meticulous refining of the commercial product. This seems rather strange, since the malodor of Propyl alcohol (or, more frequently, *iso*-Propyl alcohol) is a very common complaint against the material in various cosmetic or pharmaceutical preparations. So common, that the perfumer may have masking problems with the alcohol odor.

Although occasionally used as a solvent in perfumery work, the title alcohol finds very little use as such in perfumes.

It is used occasionally in flavor compositions, mainly in fruit flavors to introduce part of a "ripe" or "fermented" note or part of a winey flavor. The concentration is normally as low as 0.5 to 1 ppm in the finished product, actually mere traces of questionable flavor value – in the author's opinion.

The subject alcohol is considered about ten times more toxic than Ethylalcohol, and it should therefore *not* be used as a solvent for flavors.

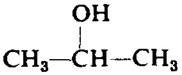
G.R.A.S. F.E.M.A. No.2928.

Prod.: the title material appears in the more advanced steps of treating Carbon monoxide with Hydrogen. It is also manufactured in the line of Petrochemical syntheses.

26-662; 66-307; 87-456; 100-862; 140-123; 160-1190; 163-66; 163-255; B-I-350;

## 2661: iso-PROPYL ALCOHOL

*2*-Propanol.
*iso*-Propanol.
*secondary*-Propyl alcohol.
Petrohol.
Dimethyl carbinol.
I.P.A.



$$CH_3-\overset{OH}{\overset{|}{C}}H-CH_3$$

$C_3H_8O = 60.10$

Colorless liquid. Sp.Gr. 0.79. B.P. 82° C.

Miscible with water, Propylene glycol, Glycerin, alcohol and most oils.

The material is flammable and its flashpoint is near room temperature. Its vapors represent an explosion hazard (at 2.5% by volume).

Alcoholic-ethereal, Acetone-like odor. The similarity to Acetone in odor is characteristic of the *iso*-Propanol, not the *n*-Propanol.

Mildly bitter-tart taste in concentrations below 5000 ppm. This concentration is many times higher than the recommended concentration in flavored products (see below).

*iso*-Propanol is widely used in pharmaceutical and cosmetic preparations sometimes simply diluted with water to a strength of about 35%, and sold as a type of "rubbing alcohol". It rarely forms part of the odorous perfume composition, but it may be used as a solvent or an auxiliary solvent. The commercial product has an objectionable odor for such purpose, and it cannot be classified as a substitute for perfumery alcohol.

The title material is used in flavor compositions to give a winey lift to various fruit flavors or introduce a mildly fermented note in Banana, Raspberry, Cinnamon, Rootbeer, Ginger, Vanilla, etc.

The concentration is equivalent to 10 to 80 ppm in the functional product.

*iso*-Propanol is considered many times more toxic than Ethylalcohol, and should therefore *not* be used as a solvent in flavor compositions.

G.R.A.S. F.E.M.A. No.2929.

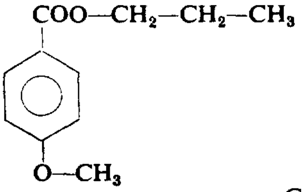
Prod.:

1) by reduction of Acetone, which comes out of Petrochemical synthesis.
2) by hydration of Propylene with Sulfuric acid or water with a catalyst. Propylene appears in the "cracking" of Petroleum.

26-662; 34-806; 66-307; 87-457; 100-579; 160-1064; 163-210; B-II-130;

## 2662: n-PROPYL ANISATE

*n*-Propyl-*para*-methoxybenzoate.



$C_{11}H_{14}O_3 = 194.23$

Colorless oily liquid. Sp.Gr. 1.08.
B.P. 280° C.

Insoluble in water, soluble in alcohol and oils.

Mild and delicately sweet, winey-floral odor of good tenacity.

Intensely sweet taste in concentrations near 20 ppm. Bitter at higher concentrations.

This ester is occasionally used in perfume compositions as part of the "powdery" odor in Cassie, Mimosa or Oriental bases, etc.

It may be used along with Anisylesters, Cinnamic alcohol, Methylionones, etc. and with Patchouli or Sandalwood oil, Oakmoss and Vetiver.

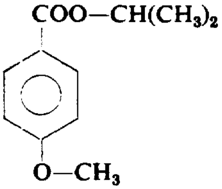
It is not a common ingredient on the shelf, and it is probably dispensable in the opinion of many perfumers.

Prod.: by azeotropic esterification of *n*-Propanol with Anisic acid.

33-62; 34-680; 163-66; 163-235;

## **2663:** iso-**PROPYL ANISATE**

*iso*-Propyl-*para*-methoxybenzoate.



$C_{11}H_{14}O_3 = 194.23$

Colorless oily liquid. Sp.Gr. 1.08.
B.P. 272° C.

Insoluble in water, soluble in alcohol and oils.

Sweet and mild, warm-floral-herbaceous odor of good tenacity.

The odor power of the material is not great, but the character is rather pleasant, suitable for Cassie and Mimosa types of "powdery" perfumes, "Crêpe de Chine" undertones, etc.

Compared to the *n*-Propylester, the title material is slightly harsher, more like Hawthorne, less refined-floral.

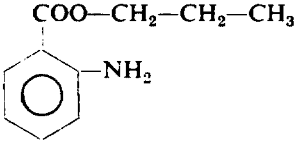
Overall, it is a material of very limited value to the perfumer, and it may as well become obsolete. It is also quite conspicuous by its complete absence from price-lists, and one may translate this as a proof of poor demand for the ester.

Prod.: by azeotropic esterification of *iso*-Propanol with Anisic acid.

103-106; 163-40; 163-211;

## **2664:** n-**PROPYL ANTHRANILATE**

*n*-Propyl-*ortho*-aminobenzoate.
This monograph includes *iso*-Propyl anthranilate, since the perfumery trade rarely discriminates between the two. The name Propyl anthranilate is commonly used for both.



$C_{10}H_{13}NO_2 = 179.22$

Colorless or very pale straw-colored liquid. Sp.Gr. 1.09. B.P. 270° C.

Insoluble in water, soluble in alcohol and oils.

Rather weak, winey, Mandarin-Orange-blossom-type odor of good tenacity.

This ester is one of the least interesting of the lower alkylesters of Anthranilic acid. It is rarely offered commercially, and it is missing from most perfume laboratories, even the well-equipped ones.

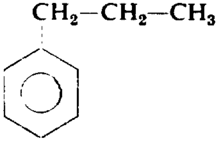
It could find some use as a modifier in floral Citrus fragrances, in support of sweet Orange oil or Mandarin oil (see Nonyl anthranilate) or as part of fruity complexes with Lactones and glycidates, etc.

Prod.: from Isatoic anhydride and Propanol (*n*- or *iso*-).

34-1011; 34-1012;

## **2665: PROPYL BENZENE**

*1*-Phenylpropane.
*n*-Propylbenzol.



$C_9H_{12} = 120.20$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 159° C.

Practically insoluble in water, soluble in alcohol and oils.

This hydrocarbon is rarely, if ever, used as such in perfumes or flavors. It has occasionally found use as a solvent for extraction of natural materials. Its boiling point is much higher than that of Benzene, and its toxicity is estimated at 50 or 100 times less than that of Benzene.

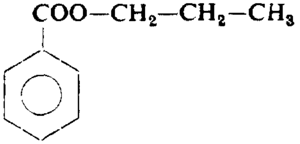
Certain natural raw materials are not satisfactorily extracted at the temperature produced in boiling Benzene, Acetone, Ethylalcohol, etc. and it may be an advantage to use a higher boiling, good solvent.

It is worth remembering that a high-boiling solvent is not necessarily more difficult to remove from the extract than a low-boiling solvent. It depends to a considerable degree upon the composition and physical effects of the extract components. Very low boiling solvents can be extremely difficult to remove from an extract, if it contains particularly good fixative matter.

Prod.:
1) from Benzyl magnesium chloride and Diethyl sulfate.
2) by reduction of Phenyl ethyl ketone or Benzyl methyl ketone.

26-662; 68-101; 68-108; 100-862; 160-840; B-V-390;
*iso*-Propylbenzene is described under the title: Cumene.

## 2666: n-PROPYL BENZOATE



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid. Sp.Gr. 1.02.
B.P. 231° C.

Insoluble in water, soluble in alcohol and oils.

Warm, deep-herbaceous-balsamic-nutlike odor of moderate tenacity.

Sweet, fruity-nutlike taste in concentrations about 30 ppm.

This ester has found a little use in perfume compositions, since it produces very pleasant complex notes with Oakmoss and Labdanum, Vetiver, etc. for new variations of Hay-like or Fougère-like fragrances, or for undertones in new types of Lavender, etc.

It is an "outdoor" type of odor, suitable for all materials of the Clover, Lavender, Hay, Fougère, Chypre, etc. and it may also be used for variations in an Ylang type of heavy floral or Oriental type.

The ester is used in flavor compositions, again partly for its nut-like effect in Hazelnut and Walnut imitation, also as a powerful undertone in fruit complexes, sometimes in wine-gum flavors, imitation Blackcurrant, etc.

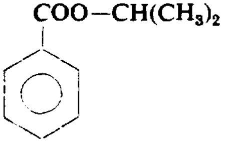
The concentration used is equivalent to about 10 to 50 ppm in the functional product.

Prod.: by azeotropic esterification of *n*-Propanol with Benzoic acid.

G.R.A.S. F.E.M.A. No.2931.

26-662; 33-621; 103-105; 160-850; 163-66; 163-235;.B-IX-112;

## 2667: iso-PROPYL BENZOATE



$C_{10}H_{12}O_2 = 164.21$

Colorless oily liquid. Sp.Gr. 1.01.
B.P. 219° C.

Insoluble in water, miscible in alcohol and oils.

Heavy-fruity, almost pungent sweet odor with floral undertone and moderate to poor tenacity. More ethereal-fruity than the *n*-Propylester.

Sweet-fruity, berry- and Plum-like taste in concentrations below 20 ppm. Not nearly as nut-like as the *n*-Propylester.

This ester is less useful in perfumes because of its greater volatility and an odor type which lends itself more to middle notes than to topnotes in a fragrance.

It is used occasionally in flavor compositions, mainly in imitation Berry flavors in trace amounts. Normal concentration may be as low as 1 ppm, but the author finds that a much higher concentration can be tolerated or, rather, that 1 ppm is barely perceptible and perhaps without effect in a berry flavor.

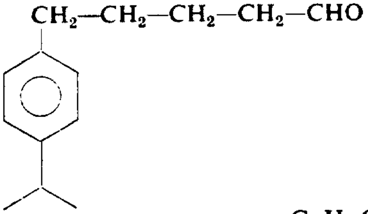
G.R.A.S. F.E.M.A. No.2932.

Prod.: by azeotropic esterification of *iso*-Propanol with Benzoic acid.

26-662; 160-850; B-IX-112;

## 2668: para-iso-**PROPYL BENZYL BUTYRALDEHYDE**

*5*-(*para-iso*-Propylphenyl)-pentanal-*1*.
Sometimes called:
Cuminyl butyraldehyde.



$C_{14}H_{20}O = 204.33$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, green-floral, diffusive and relatively tenacious odor with some resemblance to Cyclamen aldehyde, but sweeter and softer.

This aldehyde, rarely offered under its proper chemical name, does not have the power of Cyclamen aldehyde, and perhaps it is not in favor of this material at all to compare it to Cyclamal.

The subject material has been used under various trade names in perfume bases for quite a number of years. It was originally manufactured by Agfa, the German chemical company from which many interesting perfume chemicals have appeared, sometimes as a result of their research in Photochemicals, other times from Pharmaceutical research.

The aldehyde blends very well with Linalool, Geraniol, Cinnamic alcohol, Styrax, Galbanum, Geranium etc. and it has a pleasant softening effect upon Cyclamen aldehyde if that material should be used simultaneously.

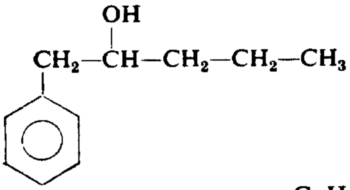
Several aldehydes, closely related to Cyclamen aldehyde, have appeared on the perfumery market during the past few years, and the title material may find some hard competition.

Prod.: from *para-iso*-Propyl phenyl butyl magnesium bromide with *ortho*-Formic ester.

The title material can be considered as a higher homologue of the chemical known as: "Cuminyl acetaldehyde".

## 2669: n-**PROPYL BENZYL CARBINOL**

*alpha*-Propyl phenylethyl alcohol.
Benzyl-*n*-propylcarbinol.
Benzyl butylalcohol.
*1*-Phenyl-*2*-pentanol.



$C_{11}H_{16}O = 164.25$

Colorless, slightly oily liquid. B.P. 247° C. Sp.Gr. 0.98.

Practically insoluble in water, soluble in alcohol and oils.

Mild-green, sweet, somewhat damp-earthy odor of moderate to good tenacity.

Tart-fruity, mildly green, sweet taste at concentrations below 10 ppm. The success of the *iso*-Propyl derivative (see next monograph) which material was marketed several decades earlier under various trade names, probably encouraged the production of this material.

And it is true that there are differences of opinion with respect to overall preference for one or the other material as a fragrance chemical.

To the author's knowledge, the title material is used only to a limited extent in fragrances today. Mainly as a supporting note in fresh-green florals, or in green-woody or green-herbaceous types. It is generally considered inferior to the *iso*-Propyl benzyl carbinol with respect to Muguet effect, but it (the title material) is excellent in new Chypre types with Oakmoss, Patchouli, Bergamot, Rose, etc.

This carbinol is also used in various types of fruit flavor, mainly as a fixative and as a mildly green note (Gooseberry, Blackcurrant, Plum, etc.). The concentration will normally be about 1 to 5 ppm in the finished product.

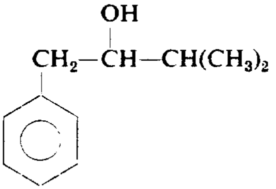
G.R.A.S. F.E.M.A. No.2953.

Prod.:
1) from Phenyl acetaldehyde plus Propyl magnesium bromide.
2) by hydrogenation of Propyl benzyl ketone.

163-235;
See also monograph: Phenyl amyl alcohol.

## 2670: iso-PROPYL BENZYL CARBINOL

Benzyl-*iso*-propyl carbinol.
*alpha*-*iso*-Propyl phenylethyl alcohol.
*1*-Phenyl-*3*-methyl-*2*-butanol.
*3*-Methyl-*1*-phenyl-*2*-butanol.



$C_{11}H_{16}O = 164.25$

Colorless, slightly oily liquid. Sp.Gr. 0.97. B.P. 238° C.

Practically insoluble in water, soluble in alcohol and oils.

Fresh-earthy-green, sweet, foliage-type odor with delicately fresh floral undertones.

This carbinol was for many years included as an important ingredient in various successful perfume specialties and bases. It is commercially available under its proper chemical name, and continuously gaining interest among the perfumers.

A common ingredient in Sweet Pea, Reseda, Lilac and Gardenia, it is also used in Rose, Clover, Honeysuckle, Violet, Jonquil, Magnolia, Jasmin, etc. or as a supporting note in Oriental fragrances. It produces very pleasant effects with Sandalwood and Geranium.

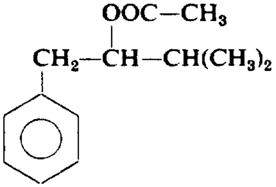
As a perfume material, it is probably more popular than the *n*-Propyl derivative (see previous monograph), while the latter is more used in flavors. The title material is, to the author's knowledge, not used in flavor compositions.

Prod.:
1) from Phenylacetaldehyde and *iso*-Propyl magnesium bromide.
2) by hydrogenation of *iso*-Propyl benzyl ketone.

34-162; 37-513; 156-76; 163-40; 163-211; 163-350;

## 2671: iso-PROPYL BENZYL CARBINYL ACETATE

Benzyl-*iso*-propyl carbinylacetate.
*alpha*-*iso*-Propyl phenylethyl acetate.
*1*-Phenyl-*3*-methyl-*2*-butanyl acetate.



$C_{13}H_{18}O_2 = 206.29$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Light, green-fruity, fresh, yet balsamic odor of moderate tenacity.

This may be one example of an Acetate, which is less interesting than its parent alcohol. It has not become nearly as popular, although it does have quite attractive, refreshingly green-fruity notes. It is an odor type of much less versatility, less compatible with the common types of fragrance bases.

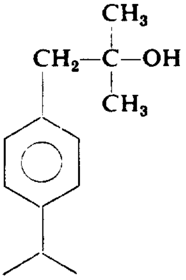
The title ester finds a little use in Rose and other floral bases.

Prod.: by azeotropic esterification of *iso*-Propyl benzyl carbinol with Acetic acid.

34-162; 163-211; 163-350;

## 2672: para-iso-**PROPYL BENZYL DIMETHYLCARBINOL**

Dimethyl cuminyl carbinol.
*3*-(*para*-*iso*-Propylphenyl)-*2*-methylpropan-*2*-ol.



$C_{13}H_{20}O = 192.30$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Refreshingly sweet-green, delicately floral and very tenacious odor.

This carbinol is very rarely offered commercially (under its proper chemical name) but it has been suggested for use in perfume compositions, mainly of Muguet, Rose, Magnolia, Mimosa, and other delicately floral, floral-green or floral-woody types.

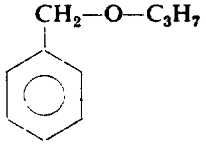
It may appear slightly sharper than Dimethylphenylethyl carbinol, and it is not quite as versatile as that very exquisite material. But it has a pleasant emphasis upon the fresh green notes which can be utilized with advantage in certain types of floral fragrance.

Prod.: from Acetone and Cuminyl magnesium bromide.

163-350;
See also monograph No. 2220.

## 2673: n-**PROPYL BENZYL ETHER**

*n*-Propyl benzyl oxide.
Benzyl-*n*-propylether.



$C_{10}H_{14}O = 150.22$

Colorless liquid. B.P. 206° C.

Practically insoluble in water, soluble in alcohol and oils.

Relatively powerful, fresh-fruity, sweet odor of moderate to poor tenacity.

The odor type and the poor tenacity speak against the use of this material in perfume compositions. It is possible that the ether is used in certain types of fragrance, e.g. light, fruity florals for detergent perfumes, etc. It is very stable in the various chemicals, usually encountered in household products, etc.

The ether has been suggested for use in flavor compositions to support fruity notes, almost any type, but the author finds that it is not nearly natural enough, even if it may be classified as a Pineapple-Pear type. The flavorist has many materials of superior effect and flavor type at his disposal today, and the title material is not recognized by the American Federal Register or F.E.M.A. Accordingly, it can not be used in imitation flavors in the USA.

The *iso*-Propyl benzyl ether (see next monograph) is slightly more interesting.

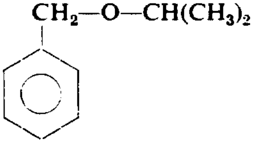
Prod.:

1) from Benzyl chloride with Propanol under alkaline conditions.
2) from Benzyl alcohol and *n*-Propanol by dehydration.

163-66;

## 2674: iso-PROPYL BENZYL ETHER

Benzyl-*iso*-propyl ether.
*iso*-Propyl benzyl oxide.



$C_{10}H_{14}O = 150.22$

Colorless liquid. Sp.Gr. 0.94. B.P. 195° C.

Insoluble in water, soluble in alcohol and oils.

Vinous-oily, fruity, relatively refreshing odor of poor tenacity.

This ether is even more volatile than the *n*-Propyl benzyl ether (see previous monograph), and it is presumably not used to any great extent in perfume compositions.

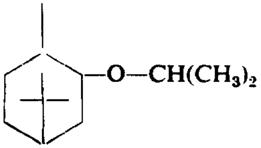
Its pleasant flavor has been utilized outside of the USA (where it is not officially permitted) in various fruit complexes, mainly as a supporting note since it is a very stable chemical. It is also used in the type of fruit flavor used in the so-called "wine-gum" which is a semi-soft gelatin candy, usually transparent and flavored with a winey fruit flavor.

Prod.:

1) from Benzyl chloride and *iso*-Propanol under alkaline conditions.
2) from Benzyl alcohol and *iso*-Propanol by dehydration.

37-171; 163-40;

## 2675: iso-PROPYL-2-BORNANYL ETHER



$C_{13}H_{25}O = 197.34$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful woody-citrusy odor of moderate to poor tenacity.

This material has been suggested for use in perfume compositions and in the reproduction of certain essential oils.

It is still too new to be discussed with sufficient experience, but the author finds reason to briefly mention this ether, since it is chemically related to several materials of Sandalwood odor and other interesting perfume chemicals.

Prod.: from Pinene via Bornyl chloride and with *iso*-Propanol in alkaline solution to the title material.

See also: *2*-Hydroxyethyl-*2*-bornanylether (monograph in this work).
*3*-Methylene-*4*-bornylbutanol is a Sandalwood material.

## 2676: n-PROPYL BUTYRATE

*n*-Propyl-*n*-butanoate.

$CH_3(CH_2)_2—OOC(CH_2)_2CH_3$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 143° C.

0.2% soluble in water, miscible with alcohol and oils.

Heavy-fruity, Pineapple-like ethereal-pungent odor of poor tenacity.

Sweet-fruity, Banana-Pineapple-like taste in concentrations below 40 ppm.

The title ester is rarely, if ever, used in perfume compositions. It could find use in certain types of cosmetic masking odors (cold wave lotions, etc. hairsprays, etc.) but there are many other materials of superior effect for such purposes.

It is used in flavor compositions, in many fruit types, such as Banana, Pineapple, Plum, Strawberry, in Rum imitations, "Tutti-frutti" flavors, Liqueur flavors, etc.

The normal concentration will be about 5 to 25 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2934.

Prod.: by azeotropic esterification of *n*-Propanol with *n*-Butyric acid, or directly with *n*-Butyric anhydride.

NOTE: Three other Propyl butyrates are described in this work, all immediately following this monograph.

## 2677: n-PROPYL-iso-BUTYRATE

*n*-Propyl-*2*-methylpropanoate.

$CH_3(CH_2)_2—OOC—CH(CH_3)_2$

$C_7H_{14}O_2 = 130.19$

Colorless liquid. Sp.Gr. 0.88. B.P. 135° C.

Very slightly soluble in water, soluble in alcohol and oils, Propylene glycol and Glycerin.

Powerful and diffusive, heavy-fruity, Pineapple type odor of poor tenacity.

Sweet, intensely fruity Apple-Pineapple-like taste in concentrations below 40 ppm.

This ester is probably not used in perfumery.

It finds some use in flavor compositions for imitation Apple, Banana, Gooseberry, Apricot, Mirabelle, Pineapple, Plum, Strawberry, etc. and will constitute about 5 to 25 ppm of the finished product.

As a flavor "ester" it is not quite as "natural" as Ethyl butyrate but not so pungent either. Relatively few Propylesters are useful as flavor chemicals, while numerous higher and lower alkyl esters are used widely in flavors.

G.R.A.S. F.E.M.A. No.2936.

It is interesting to note that the American F.E.M.A. recognizes all four isomers, separately, as flavor chemicals.

26-664; 33-732; 160-1058; 163-66; 163-235; B-II-291;

## 2678: iso-PROPYL BUTYRATE

*iso*-Propyl-*n*-butyrate.

$(CH_3)_2CH—OOC(CH_2)_2CH_3$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 130° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and diffusive, pungent, Pineapple-Strawberry type odor of poor tenacity.

Sweet-fruity, mostly Strawberry-like taste at concentrations below 40 ppm.

The title ester is apparently not used in perfumes. It finds some use in flavor composition, mainly for imitation Strawberry, Apple, Pineapple, in various berry types and fruit complexes, Tutti-frutti, etc.

The concentration will be about 10 to 40 ppm in the functional product.

The subject ester, like many other Propyl and *iso*-Propylesters, is not very popular as a flavor chemical. The lower and higher alkyl esters are generally preferred for the above types of flavor work.

G.R.A.S. F.E.M.A. No.2935.

Prod.: by azeotropic esterification of *iso*-Propanol with *n*-Butyric acid.

26-664; 33-732; 90-200; 163-40; B-II-271;

## 2679: iso-**PROPYL**-iso-**BUTYRATE**

*iso*-Propyl-*2*-methylpropanoate.

$(CH_3)_2CH—OOC—CH(CH_3)_2$

$C_7H_{14}O_2 = 130.19$

Colorless mobile liquid. Sp.Gr. 0.85.
B.P. 121° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Very diffusive, light, refreshingly fruity odor of modified Pineapple type with a Bergamot-Pear-like freshness.

Sweet-fruity, but quite refreshing, citrusy-Pineapple-like taste in concentrations below 40 ppm.

The ester is probably not used in perfumes.

It is used occasionally in flavor compositions as a modifier for higher and lower alkylbutyrates in Pineapple, Apricot, Pear and in certain types of Citrus complex flavors. It is the lightest and freshest tasting of all four Propylbutyrates.

The concentration of this ester in finished products will vary from 10 to 100 ppm.

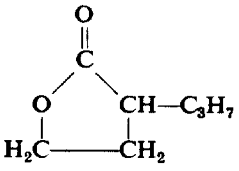
G.R.A.S. F.E.M.A. No.2937.

Prod.: by azeotropic esterification of *iso*-Propanol with *iso*-Butyric acid.

26-664; 33-732; 140-138; 160-1058; 163-138; 163-211; B-II-291;

## 2680: alpha-**PROPYL**-gamma-**BUTYROLACTONE**

*n*-Heptalactone.
Heptanolide.
*alpha*-*n*-Heptyllactone.



$C_7H_{12}O_2 = 128.17$

Colorless or almost colorless oily liquid.
Sp.Gr. 1.00. B.P. 208° C.

Practically insoluble in water, soluble in alcohol and oils.

Rather harsh-herbaceous odor, yet with sweet-herbal notes, sometimes described as the odor of grass and hay at the same time.

There seems to be general agreement that this isomer is not nearly as attractive as the *gamma*-substituted lactone (see Heptanolide). (1504).

The author is of the impression that the title material is either obsolete, or simply unavailable. In any event, there is apparently no demand for this material.

Prod.: from Ethylene oxide and *n*-Propyl malonic ester.

31-170; 156-229; 163-235;
See also: Heptanolide-*4:1*. (1504).

## 2681: iso-PROPYL CAPRATE

*iso*-Propyl decanoate.
*iso*-Propyl decylate.
*iso*-Propyl caprinate.

This monograph includes description of *n*-Propyl caprate, since the perfumery literature does not discriminate between the two esters.

$(CH_3)_2CH—OOC—(CH_2)_8CH_3$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 270° C.

Insoluble in water, soluble in alcohol and oils.

Green, vegetable-woody, oily-fruity odor, sometimes described as resembling the odor of Ho oil.

The author finds it difficult to apply this odor description, but agrees that the odor of the title material is rather complex and also strongly dependant upon the quality of the parent materials, and upon the presence (or absence) of traces of these in the ester.

This may explain why the material has not been successful as a fragrance or flavor material. It is very rarely offered commercially.

Prod.: by azeotropic esterification of *iso*-Propanol with *n*-Decanoic acid.

103-104; 163-235;

## 2682: n-PROPYL CAPROATE

*n*-Propyl-*n*-hexoate.
*n*-Propyl hexylate.
*n*-Propyl-*n*-hexanoate.

$CH_3(CH_2)_2—OOC(CH_2)_4CH_3$

$C_9H_{18}O_2 = 158.24$

Colorless liquid. Sp.Gr. 0.87. B.P. 187° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-fruity, rather heavy Pineapple-Blackberry type odor of moderate to poor tenacity.

Sweet-fruity taste of Blackberry-Plum type at concentrations near 20 ppm or lower.

The title ester is probably not used in perfume formulation.

It finds some use in flavor compositions, although the *iso*-Propyl caproate is often preferred for greater sweetness, while the title material is rather heavy, pungent-fruity. It is mostly used in imitation Pineapple, Blackberry, Plum, Cherry, etc. in concentrations equivalent to about 2 to 10 ppm in the finished consumer product.

G.R.A.S. F.E.M.A. No.2949.

Prod.: by azeotropic esterification of *n*-Propanol with *n*-Hexanoic acid.

26-664; 33-621; 34-1230; 103-104; 163-66; 163-235; B-II-323;

## 2683: iso-PROPYL CAPROATE

*iso*-Propyl-*n*-hexoate.
*iso*-Propyl hexanoate.
*iso*-Propyl hexylate.

$(CH_3)_2CH—OOC(CH_2)_4CH_3$

$C_9H_{18}O_2 = 158.24$

Colorless liquid. Sp.Gr. 0.86. B.P. 176° C.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing, sweet and almost delicately fruity odor of Pineapple-Loganberry type.

Fresh and sweet-fruity, berry-like taste in concentrations below 40 ppm.

This ester is apparently not used in perfume compositions, but it finds some use in flavors.

It is sometimes preferred over the *n*-Propyl caproate for use in imitation Pineapple, etc. The concentration of the title ester is usually higher than what is used of the *n*-Propyl ester, about 1 to 40 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2950.

Prod.: by azeotropic esterification of *iso*-Propanol with *n*-Hexanoic acid.

34-1230;

## 2684: n-PROPYL CAPRYLATE

*n*-Propyl octoate.
*n*-Propyl octanoate.
*n*-Propyl octylate.

$CH_3(CH_2)_2—OOC(CH_2)_6CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 226° C.

Almost insoluble in water, soluble in alcohol and oils.

Winey, oily-fruity, mildly Brandy-like and Berry-Grape-like odor of moderate to poor tenacity.

Fresh-fruity, winey, Berry-like taste in concentrations below 40 ppm.

This ester finds only very limited use, if any at all, in perfume compositions.

It is used occasionally in flavor compositions, and particularly in the fruit flavor type used in Gelatin candy ("Wine jelly"), and in Blackberry or Plum flavor imitations. It is also used as part of Cognac and wine flavors, Plum flavors, etc.

Prod.: by azeotropic esterification of *n*-Propanol with *n*-Octanoic acid.

26-664; 33-621; 103-104; 163-66; 163-235; B-II-348;

## 2685: iso-PROPYL CAPRYLATE

*iso*-Propyl octoate.
*iso*-Propyl octanoate.
*iso*-Propyl octylate.

$(CH_3)_2CH—OOC(CH_2)_6CH_3$

$C_{11}H_{22}O_2 = 186.30$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 217° C.

Practically insoluble in water, soluble in alcohol and oils.

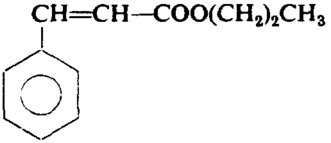
Fruity, oily, Berry-like odor of moderate to poor tenacity.

Fruity, sweet-oily, yet refreshing taste of ethereal-winey character at concentrations near 40 ppm.

The title ester is probably not used in perfume compositions, and the author believes that it is only very rarely used in flavors. It is mentioned in flavor literature, and occasionally offered commercially as a flavor ester, but it is less natural than the *n*-Propylester, and does not have any advantages over that ester.

Prod.: by azeotropic esterification of *iso*-Propanol with *n*-Octanoic acid.

## 2686: n-PROPYL CINNAMATE



$C_{12}H_{14}O_2 = 190.24$

Colorless viscous liquid, solidifying in the cold to an opaque crystalline mass. M.P. 13°C. Sp.Gr. 1.03 (liquid). B.P. 284° C.

Insoluble in water, soluble in alcohol and oils.

Sweet-and-dry, powdery-balsamic, Ambre-like slightly floral odor of good tenacity.

Sweet, deep-fruity, jam-like, balsamic taste in concentrations below 10 ppm.

This ester is used in perfume compositions, mainly in the non-floral type, and often in conjunction with Labdanum, Styrax, Anisaldehyde, etc. in variations of Fougère, Chypre, Ambre, etc. It is also used occasionally in Mimosa, Sweet Pea, Frangipanni, etc.

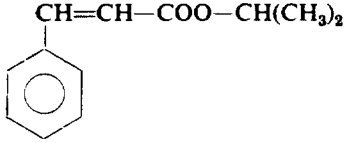
The title material is used in flavor compositions for imitation Apple, Grape, Honey and various Berry-types, Rose flavor and other "floral" flavors. It tends to produce a very "perfumey" taste at concentrations higher than 5 or 10 ppm. Normal use concentrations are just below that level, or 2 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2938.

Prod.: by azeotropic esterification of *n*-Propanol with Cinnamic acid.

34-463; 33-621; 103-105; 163-66; 163-235;

## 2687: iso-**PROPYL CINNAMATE**



$C_{12}H_{14}O_2 = 190.24$

Colorless viscous liquid. Solidifies in the cold. Sp.Gr. 1.03.

Insoluble in water, soluble in alcohol and oils. Tends to polymerize, and will become opaque, more viscous or it will jellify, and eventually become odorless.

Balsamic, sweet-and-dry Ambre type odor of good tenacity. Lighter and slightly fresher than the odor of the *n*-Propylester.

The flavor of this material is a trifle fresher, more fruity than that of the *n*-Propylester, but the difference is practically nil in a composition.

Some perfumers prefer this ester to the *n*-Propylester (see previous monograph), but there is very little difference in the effect if one considers the finished composition where the ester may be a 2% or 5% component only.

The material finds a little use in flavor compositions, mainly in imitation Raspberry, Honey, various Berry and fruit complexes, etc. The concentration will be a few ppm in the finished product.

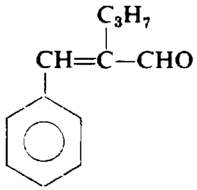
G.R.A.S. F.E.M.A. No.2939.

Prod.: by azeotropic esterification of *iso*-Propanol with Cinnamic acid.

34-462; 103-105;

## 2688: alpha-n-**PROPYL CINNAMIC ALDEHYDE**

Propylcinnamal.



$C_{12}H_{14}O = 174.24$

Pale yellowish oily liquid. Sp.Gr. 1.00. B.P. 245° C.

Insoluble in water, soluble in alcohol and oils.

Sweet, oily-herbaceous, warm and somewhat animal odor of good tenacity.

Although a pure (high olfactory grade) material actually has a pleasant odor, the title material has always had a rather bad name in perfumery, a name for being harsh and useless in fragrance compositions. It may well be that the samples available have been of poor grade or overaged. Furthermore, the perfume chemist has very little experience with this material as compared to Amyl cinnamic aldehyde, which is so important that it has been very thoroughly investigated, and its production brought to near-perfection.

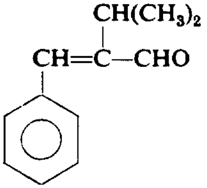
The title material could find good use in Fougères, New Mown Hay, Ambre, Lavender and many other herbaceous types. But it is rarely offered to the perfumery trade, and most often in an unacceptable grade. Consequently, the title material remains practically unknown in the average perfume laboratory.

Prod.: by condensation of Benzaldehyde with *n*-Valeraldehyde under mildly alkaline conditions.

31-51; 28-148; 156-28;

## **2689:** alpha-iso-**PROPYL CINNAMIC ALDEHYDE**

*iso*-Propylcinnamal.



$C_{12}H_{14}O = 174.24$

Pale yellowish oily liquid. Sp.Gr. 1.00.
B.P. 238° C.

Insoluble in water, soluble in alcohol and oils.

Mild and sweet Clover-like, herbaceous-warm odor of moderate tenacity. Apart from being lighter and fresher overall, it resembles the *n*-Propyl cinnamic aldehyde very much.

The title aldehyde has been suggested for use in perfume compositions as a background note in Fougères, mildly floral-herbaceous types, Lavender variations, sophisticated Pine needle fragrances, Ambre types, etc.

It blends well with Amylsalicylate, Coumarin, Oakmoss, Linalool, Anisaldehyde, etc. as well as with Methylionones, Nitromusks, Bergamot and Sandalwood, etc.

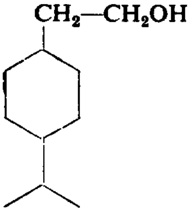
This aldehyde is, however, very rarely offered to the perfumery trade, and it is probably only made for "captive" use by a few perfume houses. Since the material is fairly well known and still not in strong demand, one may assume that it is considered more or less obsolete in perfumery.

Prod.: by condensation of Benzaldehyde with *iso*-Valeric aldehyde under mildly alkaline conditions.

31-58; 28-150;

## **2690:** para-iso-**PROPYL CYCLOHEXANE ETHANOL**

*para-iso*-Propyl cyclohexyl ethylalcohol.
*para-iso*-Propyl hexahydro phenylethylalcohol.



$C_{11}H_{22}O = 170.30$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

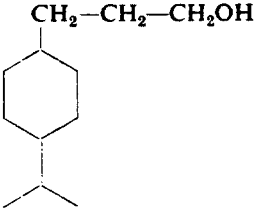
More herbaceous-woody than floral, yet relatively sweet odor of some resemblance to Linalool, yet harsher, more metallic-camphoraceous. Moderate to poor tenacity.

This material was developed in search of new and hopefully interesting alcohols related to Cuminyl alcohol and its hydrogenated derivatives. The title material could be considered as Hexahydrohomocuminic alcohol. Its odor is not very powerful and not immediately attractive. It is not versatile but it is relatively inexpensive and stable in soap. These few virtues are not sufficiently heavy on the plus side of the scale for this material, and the author believes that the title material can be considered as partly obsolete. It was probably never commercially available on a very large or continuous basis, although it was used under various trade names some years ago.

Prod.: by hydrogenation of Homo-cuminic alcohol. Other methods were also used.

## 2691: cis-para-iso-**PROPYL CYCLOHEXANE PROPANOL**

*3*-(*4*-*iso*-Propylcyclohexyl)-propan-*1*-ol.
Hexahydro-*para-iso*-propyl hydrocinnamic alcohol.



$C_{12}H_{24}O = 184.32$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

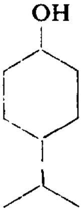
Mild, floral-balsamic, but also woody-camphoraceous odor of moderate tenacity. It is conceivable that the variations in odor, observed in the study of various samples, may be due to inevitable variations in the isomer-ratio. The *cis*-isomer is generally preferred by perfumers in the manufacturing companies.

The title alcohol has been suggested for use in perfume compositions, particularly in soap perfumes and other large-volume type fragrances. It does not seem to have maintained any great popularity, and its use is not increasing in frequency or volume. Although sold under various trade names since more than a decade ago, it appears to be on its way to oblivion.

Prod.: (several methods) e.g. by hydrogenation of *para-iso*-Propyl hydrocinnamic alcohol.

## 2692: 4-iso-**PROPYL CYCLOHEXANOL**

*para-iso*-Propyl cyclohexanol.
Dihydro cryptol.



$C_9H_{18}O = 142.24$

Colorless liquid. B.P. 210° C.

Almost insoluble in water, soluble in alcohol and oils.

Woody-camphoraceous, piney odor with semi-sweet undertones and moderate to poor tenacity.

This relatively rare alcohol has been suggested for use in perfume compositions on account of its power, low cost, and stability in soap. It has acceptable effects upon Lavender, Pine and even on Rose type fragrances for such purpose, but it needs proper blending with sweetening materials of similar volatility, e.g. Linalool, Phenylethyl alcohol, Anethole, Citronellol, esters, etc. It blends well with the conventional Fougère materials and with many of the newer Cyclohexane derivatives.

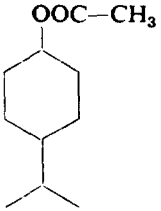
Prod.:

1) by hydrogenation of *para-iso*-Propyl phenol.
2) by electrolytic reduction of Cryptone, which can be obtained as an isolate from Eucalyptus oil fractions or certain Pine needle oils.

4-73; 67-160; 67-162; 67-211; 87-94; 89-357; 163-66; 163-40;

## 2693: para-iso-PROPYL CYCLOHEXANYL ACETATE

Dihydrocryptol acetate.



$C_{11}H_{20}O_2 = 184.28$

Colorless liquid.

Insoluble in water, soluble in alcohol and oils.

Woody-minty, sweet-camphoraceous odor with a discretely fruity note and moderate tenacity.

This ester has been suggested as a fragrance chemical, but it is rarely available, and does not seem to have any particular virtues that would make it a desirable material or preferred over the conventional materials.

Many derivatives of Cyclohexanol have powerful minty-camphoraceous and fruity odors, are inexpensive and stable, plentifully available and have already a history of testing in perfumery on their record.

The title material may be considered as almost obsolete, and it never had any great importance in perfumery.

It is produced from the corresponding tertiary alcohol (see *4-iso*-Propyl cyclohexanol).

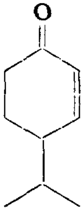
163-66;

## 2694: para-iso-PROPYL-2-CYCLOHEXENONE

Cryptone.

*4-iso*-Propyl-*2*-cyclohexen-*1*-one.

The material exists in *dextro-* and *laevo-* forms.



$C_9H_{14}O = 138.21$

Colorless liquid. Sp.Gr. 0.94. B.P. 198° C.

Practically insoluble in water, soluble in alcohol and oils.

The material polymerizes easily, increasing its viscosity and losing its odor.

Woody-minty, yet sweet-herbaceous odor of moderate to poor tenacity.

This material has been suggested for use in perfume compositions, but the author believes that the main interest in the material was based upon a temporary production of the ketone as a by-product from two Australian Eucalyptus oils (Eucalyptus polybractea and Eucalyptus cneorifolia). These oils are no longer available and no longer interesting to produce.

The title ketone could have found some use in soap perfumes on account of its power, low cost and stability in soap. If it ever became interesting again, the oil can be produced from other inexpensive starting materials (see below).

Otherwise, one may well consider the title material as practically obsolete in modern perfumery.

Prod.:

1) by isolation from certain Eucalyptus oils (see above).
2) from Nopinene and Sabinene by reaction with diluted sulfuric acid.
3) by Autoxidation of *beta*-Phellandrene.

65-388; 67-208; 67-210; 87-94; 89-355; 163-40;

## 2695: 1-PROPYL DISULFIDE

Di-*n*-propyl disulfide.

$(CH_3—CH_2—CH_2)_2S_2$

$C_6H_{14}S_2 = 150.31$

Pale yellowish mobile liquid. Sp.Gr. 0.96. B.P. 195° C.

Practically insoluble in water, soluble in alcohol and oils.

Very penetrating and powerful, diffusive odor of Garlic/Onion type, but with no lachrymatory effect. Poor tenacity. In extreme dilution more herbaceous-green than truly sulfuraceous.

The flavor is, according to well-known experiments, almost entirely dependent upon the odor impression. The reasonably pleasant level (unless you dislike Garlic very strongly) is about 0.1 ppm, but concentrations much higher are encountered in consumer products (up to 3 ppm). The minimum perceptible is much lower than 0.1 ppm.

This material is one of a number of Disulfides identified in Onion and in Garlic. It has been synthesized for the purpose of enabling the flavor chemist to make concentrated Onion and Garlic flavor for reconditioning of processed (e.g. vacuum-dried) vegetables etc.

The material is used in combination with other Sulfides, Disulfides and Trisulfides.

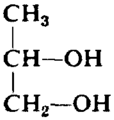
Prod.: (several methods) e.g. from Propyl iodide and Sodium thiosulfate via Sodium propyl thiosulfate, which is heated to yield the title material.

It can also be prepared from Iodine and *n*-Propylmercaptan.

66-349; 158-136; 163-374; 26-533; 61-Nov., 53; B-I-360; 105-489; 90-826;

## 2696: PROPYLENE GLYCOL

*1,2*-Propanediol.
*1,2*-Dihydroxypropane.
Methylglycol (a rather confusing, commercial name).
"P.G."



$$\begin{array}{l} CH_3 \\ | \\ CH—OH \\ | \\ CH_2—OH \end{array}$$

$C_3H_8O_2 = 76.10$

Colorless, slightly viscous liquid. Sp.Gr. 1.04. B.P. 189° C.

Miscible with water, Glycerin, alcohol and most of the common perfume and flavor oils, but not in Terpenes and many other hydrocarbons, poorly in aromatic Allyl- and Propenyl-derivatives, etc. Practically insoluble in vegetable oils and fats.

Odorless when absolutely pure.

Mild, sweet taste in aqueous solution, slightly burning or warm mouthfeel when undiluted. The aqueous solution may also leave a delayed burning feeling in the rear of the mouth.

Propylene glycol is occasionally used as a diluent in perfume compositions, but it is not considered the very best solvent for such purpose. It has practically no fixative value.

It finds very extensive use as a diluent or solvent in flavor compositions, mainly due to its low toxicity, absence of color and odor and to its mild, sweet taste. It is a fairly good solvent, although inferior to Ethyl alcohol in many respects, but it may replace alcohol in many products where alcohol tax can cause a problem.

Diluted Propylene glycol is an excellent solvent for Vanillin and Ethylvanillin. Citrus oils are poorly soluble in Propylene glycol, but partially deterpenized or terpeneless oils are usually soluble. In fact, certain types of "essence" are made by dispersing a Citrus oil in Propylene glycol, then dilute the glycol with 10-20% water and let stand for 24 hours in a cool place (most often after a 24-hour vigorous stirring period). The lower layer of the two separated liquids is then filtrated and constitutes the aroma. For certain types of household essences, Propylene glycol may be the only diluent, and the flavor may be a composition or a single flavor chemical dissolved in the glycol.

Propylene glycol has the lowest toxicity of all the common odorless glycols. However, its use is restricted in certain countries, while it is generally the only Glycol permitted for use in food flavors.

The material is used in concentrations varying from 10 ppm in Ice cream to 2000 ppm in chewing gum, while in certain syrups, it may be as high as 7000 ppm.

It is (incompletely) digested by the human digestive system, and the breakdown products are Pyruvic acid and Acetic acid.

Prod.: from Propane (obtained in Petroleum "cracking") via Propylene, with steam and Chlorine to Propylene chlorohydrin, which is saponified with Soda to Propylene glycol.

26-666; 85-65; 100-863; 104-8; 140-128; 160-1180; 163-66; 163-235; B-I-472;

## 2697: PROPYLENE GLYCOL ALGINATE

The title material is not used directly as a perfume or flavor material, but serves in food products and processed flavor products, emulsions, etc. as an emulsifier-stabilizer, usually in conjunction with emulsifiers or surfactants.

This material is used at the rate of 1000 to 50000 ppm in Ice cream, condiments, icings, dressings etc. In other words, it may constitute as much as 5% of certain (edible) food products.

The material itself is practically odorless and tasteless, although certain grades have a faintly salty taste in high concentration.

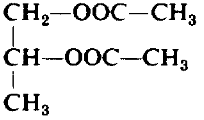
G.R.A.S. F.E.M.A. No.2941.

Prod.: from Propylene glycol and Alginic acid, which is a polymer of a *1:4*-linked *beta*-Mannuronic acid. It is obtained by extraction of certain species of seaweed, followed by acidification of the isolated Sodium alginate.

Several salts of Alginic acid are used in food industries.

See also: 100-30; 66-1322; 162-325;

## 2698: PROPYLENE GLYCOL DIACETATE



$$\begin{array}{l} CH_2{-}OOC{-}CH_3 \\ | \\ CH{-}OOC{-}CH_3 \\ | \\ CH_3 \end{array}$$

$C_7H_{12}O_4 = 160.17$

Colorless liquid. B.P. 190° C.

10% soluble in water, miscible with alcohol and oils.

Very mild fruity-acetic odor (probably spontaneous hydrolysis on mucous membranes, since very pure, acid-free esters display the same olfactory impression).

Bitter-sweet taste at concentrations higher than 200 ppm, mild and discretely fruity taste at lower concentrations. Practically tasteless below 20 ppm.

This ester has been suggested for use as a solvent and diluent in flavor compositions, since it is superior to Propylene glycol with respect to solvent properties towards terpenes and other hydrocarbons.

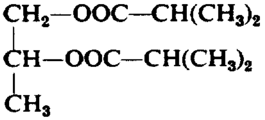
It is often used as a co-solvent to assist Propylene glycol where Citrus oils and other terpene-containing materials are used.

Its tendency to hydrolyzation is a drawback in flavor work and it is absolutely prohibitive for perfume composition work. Other and more stable esters are used in place of the title material, while a few higher alkyl esters of Propylene glycol are used in perfumery for special purposes.

Prod.: by Acetylation of Propylene glycol.

26-666; B-II-142; (private experiments).

## 2699: PROPYLENE GLYCOL DI-iso-BUTYRATE



$$\begin{array}{l}CH_2{-}OOC{-}CH(CH_3)_2\\ |\\ CH{-}OOC{-}CH(CH_3)_2\\ |\\ CH_3\end{array}$$

$C_{11}H_{20}O_4 = 216.28$

Colorless, slightly viscous liquid.

Slightly soluble in water, soluble in alcohol and oils.

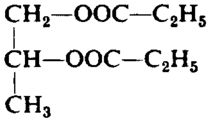
Mild, sweet-fruity, buttery odor when pure. Traces of free *iso*-Butyric acid are likely to override the odor of the material.

This ester is rarely offered commercially, since its keeping qualities are not very good. But it is manufactured by a few perfume houses for use in fragrance compositions. Smaller amounts are used in flavor compositions.

Its main purpose is that of blending with a mild, sweet, buttery or creamy note contributed to the fragrance. This note is often desirable in floral bases and is particularly suitable for Ylang-Ylang. The "mellowing" effect of this material also depends upon the composition of the fragrance, since the ester is easily hydrolyzed.

Prod. from Propylene glycol and *iso*-Butyric anhydride.

## 2700: PROPYLENE GLYCOL DIPROPIONATE



$$\begin{array}{l}CH_2{-}OOC{-}C_2H_5\\ |\\ CH{-}OOC{-}C_2H_5\\ |\\ CH_3\end{array}$$

$C_9H_{16}O_4 = 188.23$

Colorless, slightly viscous liquid.

Moderately soluble in water, soluble in alcohol and oils.

Mild, winey-fruity odor when pure, but acquires an unpleasant sour, cheesy off-odor upon improper storage or exposure to air and moisture.

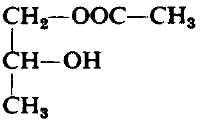
Aqueous solutions of less than 20 ppm are practically tasteless, while higher concentrations have mild fruity taste, winey taste or, beyond 500 ppm, bitter-fruity taste.

The title ester has found some use in perfume compositions and occasionally in flavor compositions. It is rarely offered commercially, but normally manufactured by the interested party for "private" use. The ester may hydrolyze under certain, not necessarily abnormal, circumstances, and it is not very popular among perfumers for that reason. Its mission in perfumes is mostly that of "mellowing" and introducing notes simulating well-aged alcoholic perfume solutions. It is often used in conjunction with Ethyl acetoacetate and similar materials for such purpose.

Prod.: from Propylene glycol and Propionic anhydride.

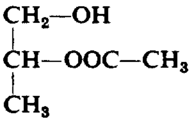
## 2701: PROPYLENE GLYCOL MONOACETATE

Commercial products may be mixtures of the so-called *alpha-* and *beta-*Monoacetates (*primary-* or *secondary-*), while it is possible to manufacture one or the other isomer in fairly pure form.



$$\begin{array}{l}CH_2{-}OOC{-}CH_3\\ |\\ CH{-}OH\\ |\\ CH_3\end{array}$$

*alpha-*



$$\begin{array}{l}CH_2{-}OH\\ |\\ CH{-}OOC{-}CH_3\\ |\\ CH_3\end{array}$$

*beta-*

$C_5H_{10}O_3 = 118.14$

Colorless, slightly viscous liquid. Sp.Gr. 1.06. B.P. 183° C.

Moderately soluble in water, soluble in alcohol and oils.

Mildly fruity-ethereal-acetic odor.

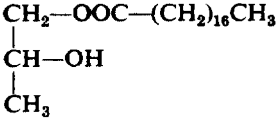
Aqueous solutions of less than 20 ppm are virtually tasteless, while a mildly sour-winey-fruity taste is perceptible at higher levels, and a more bitter taste appears at levels beyond 1000 ppm.

This ester is sometimes used in flavor compositions as an auxiliary solvent and diluent for flavor materials or for the entire composition. It has some tendency of hydrolyzing, producing a more acetic note, while overall, it is more stable than the Di-acetate in this respect.

B-II-142; 158-165; 26-666;

## 2702: PROPYLENE GLYCOL STEARATE

Propylene glycol mono stearate.
Propyleneglycol mono-octadecanoate.



$$\begin{array}{l} CH_2{-}OOC{-}(CH_2)_{16}CH_3 \\ | \\ CH{-}OH \\ | \\ CH_3 \end{array}$$

$C_{21}H_{42}O_3 = 342.57$

The above formula describes the *alpha*-monostearate.

White or colorless silky crystals or crystalline powder.

Virtually odorless when pure, but commercial material normally carries a mild, warm-oily, bland odor.

Fatty-oily, bland taste. Gives practically no taste to water at trial concentrations of 1000 ppm.

The title ester is not a flavor material but it is recognized as a permitted food additive, particularly used in shortening for cakes and bread. The normal use-level is about 15 % of the surfactants in the shortening, or about 1.5 % in the total shortening.

Used in conjunction with other approved emulsifiers and surfactants, it assists in producing better "aeration" of the bread or cake during the baking process.

The material has interest to the flavorist in the fact that it acts as a fixative upon most flavor compositions. In the emulsion type of shortening, the flavor may be incorporated in the fat-and-oil phase of the shortening, according to composition of the flavor. The title material is soluble in vegetable oil in the proportions normally required.

G.R.A.S. F.E.M.A. No.2942.

Normal level in finished products: from 5000 to 100000 ppm in baked goods, toppings and candy. In other figures, the material may constitute up to 10 percent of certain finished goods.

162-432; 162-441;

## 2703: iso-PROPYL ETHER

Di-*iso*-propylether.
Di-*iso*-propyl oxide.

$(CH_3)_2CH{-}O{-}CH(CH_3)_2$

$C_6H_{14}O = 102.18$

Colorless mobile liquid. Sp.Gr. 0.72. B.P. 69° C.

0.2 % soluble in water, soluble in alcohol, miscible with oils.

Ethereal, sweet, nauseating and very diffusive odor. The vapors are flammable and produce explosive mixtures with air at room temperature. Mixtures as low as 1 % of the vapors of title material in air represent explosion hazard.

The subject ether is sometimes used as an extraction solvent in the preparation of perfume and flavor materials from natural raw materials. Since it is always possible that traces of the solvent are left in the extract, the perfumer should also know the odor of this and similar solvents.

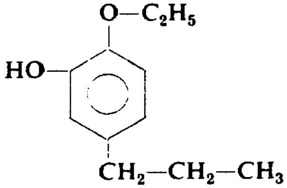
The author believes that the title material is not used in perfumes or flavors as such.

Prod.: by dehydration of *iso*-Propanol.

26-532; 37-176; 163-40; B-I-362; Shell data sheet 9/1957.

## 2704: 5-PROPYL-2-ETHOXYPHENOL

"Dihydro vanitrope".
*3*-Hydroxy-*4*-ethoxy propylbenzene.
*1*-Ethoxy-*2*-hydroxy-*4*-propylbenzene.
"Homodihydro eugenol".
*para*-Propylcatechol ethylether.



$C_{11}H_{16}O_2 = 180.25$

White crystals. Insoluble in alcohol, soluble in alcohol and oils.

Warm and very sweet balsamic, Nut-like and Vanilla-like odor, but not nearly as powerful as Vanitrope. Excellent tenacity.

The title material has been suggested for use in perfume compositions mainly because of the assumption that the absence of the Propenyl group should greatly reduce the hazard of skin-irritation, usually ascribed to that particular group. There is still a Phenol group - like in many of the Salicylates, also accused of being irritating.

If it is true that this material is much safer in cosmetic use, there is good reason to promote the further application of it in creative perfumery. It will probably not be interesting for the flavorist, because it lacks Vanilla flavor power, and it is far too expensive as a flavor material calculated upon the yield of Vanilla flavor supplied by the title material.

As a novel type fixative in Oriental fragrance types, as a support to spicy-woody fragrance types, in combination with Patchouli, Styrax, Oakmoss, etc., it has good possibilities, and its versatility makes it an interesting material for "unconventional" creative perfumery.

Prod.: by selective hydrogenation of Vanitrope (see Propenyl guaethol).

Also by hydrogenation of *iso*-Safrole, treatment of the Dihydro-*iso*-safrole with Phosphorous pentachloride, followed by hydrolysis and finally Ethylation of the resulting *4*-Propenylcatechol to the title material.

See also: Dihydro eugenol (944), and
Methyl dihydroeugenol (2000).

156-379;

## 2705: n-PROPYL FORMATE

*n*-Propyl methanoate.

$CH_3—CH_2—CH_2—OOC—H$

$C_4H_8O_2 = 88.11$

Colorless mobile liquid. Sp.Gr. 0.90.
B.P. 81° C.

3% soluble in water, miscible with alcohol, Propylene glycol and oils.

Powerful and diffusive, ethereal, heavy, almost nauseating odor.

Fruity, Rum-like or Arak-like taste in concentrations below 100 ppm. The taste has sometimes been classified as "Zlivovitz-like" (a Plum-Brandy of great popularity in Eastern and Southeastern Europe).

The material is flammable and its vapors form explosive mixtures with air.

This ester is probably not used in perfume compositions, except in rare cases of application in Cologne topnote compositions, etc.

It finds some use in flavor compositions, such as imitation Apple, Rum, Lemon, Orange, Plum, etc., and in many types of Berry flavor. The concentration in the finished product may be about 20 to 100 ppm.

G.R.A.S. F.E.M.A. No.2943.

Prod.: by reacting *n*-Propanol with Formic acid in the presence of anhydrous Calcium chloride.

Also by azeotropic esterification.

26-664; 33-621; 103-83; 100-864; 140-131; 160-1002; 163-66; 163-235; B-II-21;

## 2706: iso-PROPYL FORMATE

*iso*-Propyl methanoate.

$(CH_3)_2CH—OOC—H$

$C_4H_8O_2 = 88.11$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 70° C.

2% soluble in water, miscible with alcohol, Propylene glycol and oils.

Sweet-ethereal, very diffusive odor, fresher than Chloroform, not as pungent as *n*-Propylformate.

Sweet-ethereal, slightly "fermented-fruity" taste in concentrations below 200 ppm. Slightly burning mouthfeel at higher concentrations.

This ester finds some use in flavor compositions, mainly in Berry complexes and in imitation Melon (assists in the diffusive-ethereal aroma picture). In fact, it is characteristic of this ester, that it is very suitable for Melon, while the *n*-Propylester is not so.

The title material has insecticide properties.

The concentration of this ester in finished products will normally be about 20 to 100 ppm.

The author is not aware of any significant use of this ester in perfumes, except occasional use in Colognes to emphasize the lift, normally supplied by the alcohol in the finished solution.

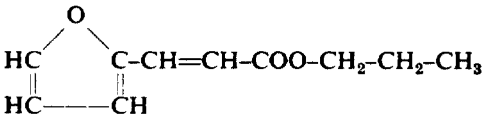
G.R.A.S. F.E.M.A. No.2944.

Prod.: by azeotropic esterification of *iso*-Propanol with Formic acid.

26-664; 103-83; 140-132; 160-1002; B-II-21;

## 2707: PROPYL-2-FURANACRYLATE

Propyl-*3*-(*2*-furyl)-acrylate.



$C_{10}H_{12}O_3 = 180.21$

Pale yellowish or almost colorless liquid.
Sp.Gr. 1.05. B.P. 236° C.

Almost insoluble in water, soluble in alcohol and oils.

Light, fruity, Strawberry-Applepeel and Pear-like odor of moderate to poor tenacity.

Fresh, fruity-caramellic, sweet taste in concentrations below 40 ppm. Rather bitter at higher concentrations.

The title ester is apparently not used in perfumes.

This material finds limited use in flavor compositions, and, in spite of its overall fruity character, it is most suitable for Honey, Nut and Coffee compositions, where its intense sweetening effect comes to use.

The concentration in finished products is about 0.1 to 5 ppm.

The material tends to discolor under exposure to daylight, and this may be one of the reasons for its limited popularity.

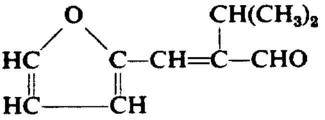
Prod.: by azeotropic esterification of *n*-Propanol with Furanacrylic acid.

G.R.A.S. F.E.M.A. No.2945.

163-211; 163-235;

## 2708: alpha-iso-PROPYL FURFURACROLEIN

*2-iso*-Propyl-*3*-(*2*-Furyl)-*2*-propen-*1*-al.



$C_{10}H_{12}O_2 = 164.21$

Yellowish oily liquid. Sp.Gr. 1.03.
B.P. 229° C.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant, oily-woody, herbaceous-green odor of moderate to poor tenacity.

This aldehyde has been suggested for use in perfume compositions, but it is rarely offered commercially under its proper chemical name.

It was developed in a series of research experiments with Furfural and alifatic aldehydes, parallel to the more successful line from Benzaldehyde and alifatic aldehydes. A few of these alkyl-substituted Furfuracroleins have found use in perfumes, some also in flavors.

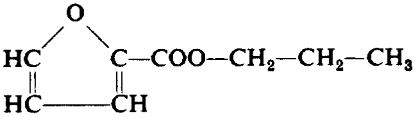
The title aldehyde gives very pleasant and interesting effects with herbaceous-floral materials, including Jasmin and Mimosa, or with Amylsalicylate in novel types of Fougère.

Prod.: from Furfural by condensation with *iso*-Valeric aldehyde under mildly alkaline conditions.

31-40; 91-151;

## 2709: n-PROPYL FUROATE

Propyl-*2*-furoate.
*n*-Propyl pyromucate.
Furan-*alpha*-carboxylic acid, *n*-Propylester.



$C_8H_{10}O_3 = 154.17$

Colorless liquid. Sp.Gr. 1.07. B.P. 211° C.

Very slightly soluble in water, soluble in alcohol and oils.

Peculiar sweet-oily, herbaceous-earthy odor of moderate to poor tenacity.

Sweet, warm, oily-herbaceous, caramellic-earthy taste in concentrations below 5 ppm. Heavy-earthy, but still sweet at concentrations near 20 ppm.

This ester finds some use in flavor compositions, mainly in Chocolate and Mushroom imitation flavor, where the deep-warm, herbaceous-nutlike flavor adds power and character. It blends quite well with the more conventional Amylphenylacetate and similar esters for above purposes, and it is also compatible with *1*-Octen-*3*-ol (see Amyl vinyl carbinol).

The concentration of this material in finished consumer products will normally be as low as 0.05 to 0.30 ppm. It is particularly low in Chocolate flavor, which is a very sensitive flavor, or rather, a flavor to which the buying clientèle is critically sensitive and alert.

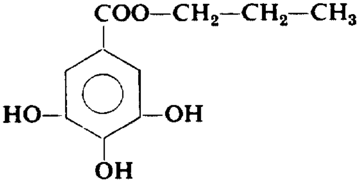
G.R.A.S. F.E.M.A. No.2946.

Prod.: by azeotropic esterification of *2*-Furoic acid with *n*-Propanol.

26-664; B-XVIII-275;

## 2710: n-PROPYL GALLATE

"Tenox P.G." (Eastman Chem. Co.).
Progallin.



$C_{10}H_{12}O_5 = 212.21$

Almost white, but commonly off-white or greyish microcrystalline powder or small crystals.
M.P. 150° C.

0.3% soluble in water, 50% soluble in alcohol, 1% soluble in most vegetable oils.

Practically odorless when pure, but some commercial products may carry a faintly dry-medicinal odor.

Aqueous solutions of higher than 10 ppm concentration have a perceptibly bitter taste, or bitter-metallic taste and mouthfeel. The material is tasteless in the concentrations recommended for finished products.

This ester is not an active flavor or perfume material, but it serves as an important Antioxydant in many food products and flavor concentrates. It is also used to some extent in essential oils to retard oxidation of Monoterpenes and sensitive aldehydes or ketones, etc. See also monographs: Butyl hydroxy anisole and Butyl hydroxy toluene. The title material is often used in conjunction with the two named materials, and with Citric acid or similar acid as booster/synergist.

The subject ester suffers from the same drawback as other Antioxidants, in the fact that it is a phenol. It discolors in contact with Iron and upon prolonged exposure to air and daylight. The latter type of discoloration may not take place at the low concentration normally used. Only one Antioxidant of importance in food is not a phenol (Ethoxy dihydro trimethyl quinoline).

Propyl gallate is used at the rate of 0.03 to 1 ppm in finished products, mostly in combination as outlined above.

Lemon, Lime, Fruit and Spice flavors are also often treated with this material.

G.R.A.S. F.E.M.A. No.2947.

The American Food and Drug Administration has approved its use and limited the amount to 200 ppm based upon the fat or oil matter present in the consumer product which is treated. The material may be used in freeze dried meats and sausages in the amount of 100 ppm. A further addition of 100 ppm of other Antioxidants is permitted. These figures are based upon the weight of the fat only – in the meat or sausage.

100-864; 162-225; 162-236;

## 2711: n-PROPYL HEPTOATE

Propyl heptylate.
Propyl heptanoate.
Propyl oenanthate (misleading and abandoned name).

$CH_3—CH_2—CH_2—OOC(CH_2)_5CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 206° C.

Almost insoluble in water, soluble in alcohol and oils.

Green-fruity, winey, slightly fatty odor of rather poor tenacity. The fruity notes resemble the odor of juice from green Grapes (also called white grapes).

Tart-fruity, winey, mildly oily-green taste in concentrations below 40 ppm. Not very pleasant at higher levels.

This ester, like most other Propylesters, is used only rarely in flavors. Generally speaking, the Propylesters lack natural character and immediately attractive aroma, while there are many such esters of quite pleasant odor.

It finds use in imitation Apple, Coffee, Cognac, Rum, Grape, and in various berry complexes, Tutti-frutti types, etc.

The use level is equivalent to about 5 to 20 ppm in the finished product.

There is only very little use of this ester in perfumery. It may find use as part of imitation Cognac oil and other materials for "winey" topnotes, and in Geranium compositions, Ylang, etc. where the Brandy-winey character can be of interest.

Prod. by azeotropic esterification of *n*-Propanol with *n*-Heptanoic acid.

G.R.A.S. F.E.M.A. N.2948.

33-621; 35-61; 103-104; 163-235;

## 2712: iso-PROPYL-n-HEPTOATE

*iso*-Propyl heptylate.
*iso*-Propyl heptanoate.
*iso*-Propyl oenanthate (misleading and abandoned name).

$(CH_3)_2CH—OOC(CH_2)_5CH_3$

$C_{10}H_{20}O_2 = 172.27$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 195° C.

Almost insoluble in water, soluble in alcohol and oils.

Ethereal-fruity, mildly green, Grape-juice-like or Apple-like odor of poor tenacity.

Refreshing, fruity-green, vinous taste at concentrations below 40 ppm. Lighter, more ethereal than the *n*-Propylester.

The title ester is rarely used in perfumes.

It finds a little use in flavor compositions for imitation Apple, Grape, Coffee, Gooseberry, Melon, etc. but the concentration is normally mere traces.

Prod.: by azeotropic esterification of *iso*-Propanol with *n*-Heptanoic acid.

The title material is not specifically mentioned in the American G.R.A.S. list, but the *n*-Propylester is included (see previous monograph).

163-66; 163-235;

## 2713: PROPYL HEPTYL ETHER

*n*-Heptyl-*n*-propylether.

$CH_3—CH_2—CH_2—O—(CH_2)_6CH_3$

$C_{10}H_{22}O = 158.29$

Colorless mobile liquid. Sp.Gr. 0.79.
B.P. 187° C.

Almost insoluble in water, soluble in alcohol and oils.

Fruity, rather bland, mellow odor of poor tenacity. Not as green as the odor of the *iso*-Propyl heptylether (see next).

This ether has been suggested for use in perfumes and flavors, but it does not seem to have achieved much popularity. It could be used in masking odors for industrial purposes, and it may also find some use in fruity flavor compositions except in the USA where it is not included in the G.R.A.S. list, and therefore not permitted for use in food flavors.

Prod.: from Sodium propoxide plus *n*-Heptyl chloride, preferably in presence of a Sodionaphthalene type catalyst.

37-176; 66-321; 163-66;

## 2714: iso-PROPYL HEPTYLETHER

*n*-Heptyl-*iso*-propylether.

$(CH_3)_2CH—O—(CH_2)_6CH_3$

$C_{10}H_{22}O = 158.29$

Colorless mobile liquid. Sp.Gr. 0.78.
B.P. 173° C.

Practically insoluble in water, soluble in alcohol and oils.

Green-fruity, ethereal odor, often described as resembling the odor of unripe (green) Mountain ash berries (fruits of Sorbus aucuparia in Europe or the related Sorbus Americana in North America).

The subject ether has been suggested for use in perfume compositions and it may occasionally find some use, although it is a rare and not truly needed material.

Its peculiar fresh, tart green odor is useful in certain topnote compositions, but it needs considerable work, since it lacks naturalness and softness. Amylsalicylate will tone it down, but detracts from its effect as a topnote material. A careful selection of Citrus oils or compositions of Hexenyl esters with Linalool etc. may produce attractive notes with this material.

Prod.: from Sodium-*iso*-propoxide and *n*-Heptyl chloride in presence of a Sodionaphthalene type catalyst.

163-40;

## 2715: n-PROPYL HEPTYL KETONE

*4*-Undecanone.
Heptyl propyl ketone.

$CH_3-CH_2-CH_2-CO-(CH_2)_6CH_3$

$C_{11}H_{22}O = 170.30$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Very fruity, pungent-oily odor of moderate to poor tenacity. It is more fruity than Ethyl octyl ketone (*3*-Undecanone) and still more fruity than Methyl nonyl ketone (*2*-Undecanone).

The subject ketone has been suggested for use in perfume compositions, but it does not appear in price lists, and is rarely found on the perfumer's shelf. The material has very little to offer of real interest to the perfumer (or flavorist), and only if the ketone could be made available at very low cost and in abundance, there would be some reason to test it further for its possible inclusion in certain types of compositions. Briefly, the author believes that the title material can be considered as practically obsolete.

Prod.: from Heptylmalonic diethylester plus *n*-Propyl bromide.

31-81;

## 2716: iso-PROPYL-n-HEPT-1-YNE CARBONATE

*iso*-Propyl octynoate.
*iso*-Propyl heptin carbonate.

$(CH_3)_2CH-OOC-C\equiv C-(CH_2)_4CH_3$

$C_{11}H_{18}O_2 = 182.27$

Colorless oily liquid. B.P. 224° C.

Insoluble in water, soluble in alcohol and oils.

Powerful and penetrating, rather sharp-green, leafy odor of moderate to poor tenacity. Not as sweet as Methyl octin carbonate, and not as natural as Amyl heptin carbonate.

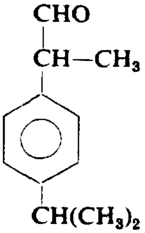
The title acetylenic ester seems to be one of those "intermediate" type odorants, deficient in character, and failing in competition with related, but more conventional materials. There is no strong reason to put such material on the perfumer's shelf, and it may as well remain in the research cabinet among the thousands of chemicals manufactured on experimental scale subsequent to the success of a new perfume chemical. However, the time it takes before a new chemical strikes success, is often so long, that many derivatives are brought out in the market while the perfumers are still undecided in their experiments with the first chemical; such flooding adds to the general confusion and may extend the delay before the selected material becomes financially successful.

Prod.: basically from Castor oil, via Heptaldehyde to Heptyne, from which the acid and finally the ester is produced.

5-245;

## 2717: para-iso-PROPYL HYDRATROPIC ALDEHYDE

*para-iso*-Propyl-*alpha*-methyl phenylacetaldehyde.
*para-iso*-Propyl hydratropal.
*para-iso*-Propyl-*alpha*-phenylpropionic aldehyde.



$C_{12}H_{16}O = 176.26$

The commercial product usually contains some *meta*-isomer (see below: Prod.).

Colorless liquid. Viscosity increases upon exposure to air, while the odor intensity decreases.

Insoluble in water, soluble in alcohol and oils.

Powerful, refreshingly green, sap-like or "twig-like" odor with a pungent (unless diluted) herbaceous character, yet overall sweet, slightly woody and rather heavy. In proper dilution the odor becomes similar to that of Willow leaves.

This aldehyde, commercially available for many years already, has only very slowly gained foothold on the perfumer's shelf, in spite of the excellent results and record of success already attributed to this material. Variations in quality of material from different suppliers, relatively poor shelf stability, etc. may be some of the reasons for apparent reluctance on the part of the perfumers in general to use this material.

In combination with delicately woody odors, Methylionones and refined Cedarwood-derivatives, Sandalwood and many carbinols, it performs very well. Styrax and Oakmoss are excellent blenders for the aldehyde, and Galbanum an interesting companion.

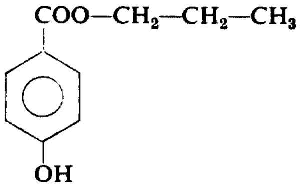
However, high quality and uniformity in manufactured lots are prerequisites for the further success of such material. It could become one of the important aldehydes.

Prod.: from *para-iso*-Propyl acetophenone (see Acetocumene) via the Glycidate synthesis (Darzens). Acetocumene will often contain considerable amounts of *meta*-isomer, and this is where one serious impurity may enter the odor picture.

156-296; 163-350; See also 2741.

## 2718: PROPYL-para-HYDROXYBENZOATE

*para*-Hydroxy propyl benzoate.
"Nipasol".
"Propyl parasept".
"Propyl paraben".
"Tegosept gamma".



$C_{10}H_{12}O_3 = 180.21$

White or colorless crystals. M.P. 97° C.

0.05% soluble in water, soluble in alcohol and most oils.

The solubility in water is sufficient (500 ppm) to accomplish effective fungistatic action.

This material is virtually odorless, and the (above mentioned) aqueous solution is practically tasteless.

It is mentioned in this work because it is a relatively important preservative and fungistat in food products and flavor compositions (prepared, diluted flavors, etc.).

The concentration used in beverages, candy, baked goods etc. is about 30 to 100 ppm, while in Ice cream the concentration may be as high as 130 ppm. Higher concentrations are rarely found in functional (consumer) products.

The Methyl ester is commonly used in pharmaceutical preparations, while the Ethylester is less common in use. The title material is one of the most effective of this type of fungistat. It will prevent growth of fungus and yeast, but it will not eliminate already existing spores or kill grown fungi. In other words, it will protect a "clean" product from contamination of growing microorganisms, but the effect has its limits.

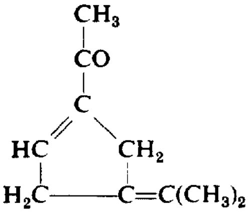
Prod.: Potassium salicylate yields by heating *para*-Hydroxybenzoic acid, from which the esters are prepared by conventional methods.

G.R.A.S. F.E.M.A. No.2951. Note: the maximum concentration by FDA is set at 100 ppm in the finished product.

100-864; 163-66; 163-71; 162-144;

## 2719: iso-PROPYLIDENE-3-ACETYL-1-CYCLOPENTENE-5

*3-iso*-Propylidene-*1*-acetylcyclopent-*5*-ene.
"Eucalyptus ketone".



$C_{10}H_{14}O = 150.22$

Pale yellowish or almost colorless oily liquid. Sp.Gr. 0.95. B.P. 227° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, warm-herbaceous odor, sweeter, but also sharper than Carvone, but with some resemblance to that ketone. The tenacity is rather poor.

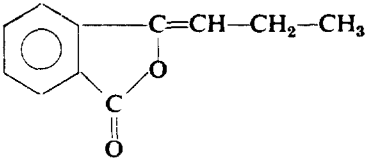
The chemist has been tempted to compare this ketone to the Jasmones, but the perfumer will find little resemblance. The tenacity is much inferior, the floral character is practically non-existing, but there is a similarity in the spicy warmth only. Since the material exists in Nature, it has come into the field of interest of the perfume chemists, but there is apparently no sincere interest from the side of the perfumer in this ketone. If it were made available at very low cost, it could undoubtedly find use in everyday perfumery.

However, its Acetylgroup presents a perceptible hazard in producing sour-acetic notes under certain circumstances in functional products (compare Acetylindane musks, etc.).

Prod.:
1) by isolation from Eucalyptus globulus oil (Spanish).
2) it has also been prepared synthetically.

34-579; 89-266; 163-211;

## 2720: 3-PROPYLIDENE PHTHALIDE



$C_{11}H_{10}O_2 = 174.20$

Colorless or very pale straw-colored, slightly viscous liquid. Sp.Gr. 1.08. B.P. 273° C.

Powerful, very warm, spicy-herbaceous odor of good tenacity.

Warm, but not pungent, spicy-herbaceous, condiment-like taste in concentrations below 10 ppm. The minimum perceptible is far below 1 ppm.

This lower homologue of Ligusticum lactone (see *n*-Butylidene phthalide) has found use in flavor compositions, mainly in meat flavors and spice blends, flavors for condiment and seasonings, sauces etc. It is also occasionally used as background note in heavy fruity types, such as Plum, Mango, etc.

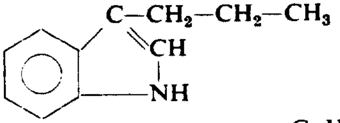
The concentration in finished consumer products may be as high as 5 ppm, but the explanation for this high level is probably in the fact that the material is used in products, consumed in small amounts, such as seasonings, sauces, spice blends, etc.

The author is not aware of any significant use of the title lactone in perfume compositions, although interesting combinations with Oakmoss and Opopanax can be made with this material.

G.R.A.S. F.E.M.A. No.2952.

Prod.: from Sodium butyrate plus Butyric anhydride and Phthalic anhydride.

## 2721: beta-n-PROPYL INDOLE



$C_{11}H_{13}N = 159.23$

Colorless or pale yellowish liquid when freshly prepared. Becomes darker upon exposure to daylight and air.
B.P. 260° C.

Practically insoluble in water, soluble in alcohol and oils.

Penetrating, dry odor with faintly fecal note and usually also a naphthalenic odor. Overall not pleasant, not even in dilution.

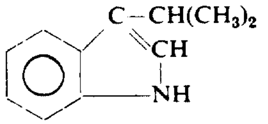
This Indole-derivative, one of the liquid types, has been suggested for use in perfume compositions as a modifier for Indole and Skatole. However, in the purity so far offered commercially, the material would not have much chance of becoming popular. If the fecal-naphthalenic notes are indigenous to the chemical, one may as well consider this Indole as generally unacceptable by the perfumers.

Prod.: from Valeraldehyde-phenylhydrazone by heating with Zinc chloride.

163-235;

## 2722: beta-iso-PROPYL INDOLE

*3-iso*-Propyl indole.



$C_{11}H_{13}N = 159.23$

Colorless or pale amber-colored liquid.
B.P. 288° C.

Insoluble in water, soluble in alcohol and oils.

Penetrating and heavy, but in dilution floral, sweet-animal odor of good tenacity.

The odor is often compared to that of 7-Methyl quinoline.

This Indole has been available and was suggested for use in perfume compositions. It may be used in trace amounts in Lilac, Jasmin, Narcisse, etc. or it may constitute part of an artificial Civet base. It has also been used in Ylang compositions and various exotic, heavy florals.

It is rarely offered commercially, but may appear as part of perfume specialties and bases.

Prod.: from *iso*-Valeraldehyde-phenylhydrazone plus Zinc chloride.

69-84; 163-211;

## 2723: n-PROPYL MERCAPTAN

*n*-Thiopropyl alcohol.
*n*-Propane thiol.

$CH_3—CH_2—CH_2—SH$

$C_3H_8S = 76.10$

Colorless liquid. Sp.Gr. 0.82. B.P. 68° C.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Very powerful, penetrating and diffusive, Cabbage-like, sulfuraceous odor, unpleasant unless extremely diluted.

Concentrations below 1 ppm have a sweet Onion-Cabbage-like, not unpleasant taste.

The title material is probably not used in perfume compositions.

It finds some use in flavor compositions, mainly in Onion flavors, but also in various fruity types, where minute traces of this Mercaptan can introduce quite natural effects.

Concentration is normally about 0.1 to 0.5 ppm in the finished product.

Prod.:

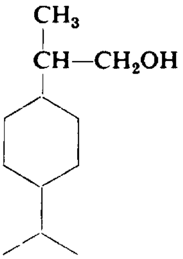
1) from *n*-Propyl chloride and Potassium hydrosulfide.
2) from *n*-Propanol plus Bromine and red Phosphorus in presence of Sodium sulfate.

G.R.A.S.

66-347;

## 2724: para-iso-**PROPYL**-beta-**METHYLCYCLOHEXANE ETHANOL**

*beta*-Methyl hexahydro homocuminic alcohol.
Hexahydro-*para-iso*-propyl hydratropic alcohol.



$C_{12}H_{24}O = 184.32$

Colorless, slightly viscous liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Mild, floral-woody odor, remotely rosy-balsamic, and of moderate tenacity.

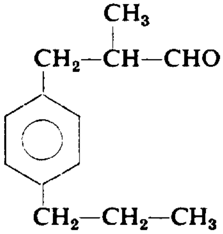
This alcohol has been suggested for use in perfume compositions, and it has been of some use in soap perfumes, etc. However, it is not truly inexpensive and has not been available in very large quantity. It dates back to the 1950's at a time when Linalool and many common alcohols were still relatively expensive for soap use. Today, it falls behind in competition with the abundance of low-cost powerful odorants, many with very attractive odors.

The material may be considered as partly obsolete.

Prod.: by hydrogenation of *para-iso*-Propyl hydratropic alcohol.

## 2725: para-n-**PROPYL METHYLHYDROCINNAMIC ALDEHYDE**

*para-n*-Propyl-*alpha*-methyl phenylpropionic aldehyde.
"*iso*-Cyclamal".
(the *iso*-Propyl derivative is Cyclamen aldehyde.



$C_{13}H_{18}O = 190.29$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Although the odor of this aldehyde is not as fresh-powerful, penetrating and diffusive as that of Cyclamen aldehyde, there is considerable similarity in the odor of the two. The title aldehyde has superior tenacity, but does not perform as well in the initial notes in a composition. It seems less green-fresh. One might suspect that since this aldehyde is "the rare one", less attention has been paid to the development of olfactory pure material, and fewer samples have been submitted to perfumers for comments. Briefly, the material has not been promoted, perhaps with reason.

It is rarely offered commercially, and apparently not in demand.

Prod.:

1) from *para-n*-Propylbenzaldehyde plus Propionic aldehyde, followed by hydrogenation.
2) from *para-n*-Propyl benzaldehyde plus Methyl malonic ester and Sodium ethoxide, followed by saponification of the resulting ester, removal of the alcohol, acidification to release the acid, decarboxylation to produce the new acid, from which the title aldehyde is produced with Formic acid in gas form.

## 2726: iso-PROPYL MYRISTATE

*iso*-Propyl tetradecanoate.
"Deltyl extra" (Givaudan). The title material is main component, while the – laurate and the – palmitate are minor components of that specialty.

$(CH_3)_2CH—OOC(CH_2)_{12}CH_3$

$C_{17}H_{34}O_2 = 270.46$

Colorless oily liquid, solidifying in the cold, melting at 5° C. Sp.Gr. 0.85. B.P. 305° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Virtually odorless when pure, or displaying only a very faint, flat oily-fatty, but *not* rancid odor.

Many commercial lots have variable amounts of rancid or overly fatty odors, repulsive sulfuraceous by-notes, etc. Such materials are unsuitable for perfumery and cosmetic purposes.

The title ester has no positive application as a fragrance material or a flavor ingredient, but it is widely used as a diluent, a plasticizer and a skin-emollient. The concentration of the title material in a functional product to be used "as such" by the customer may be as high as 80% or more, while 40 to 50% is quite common. The olfactory quality of the subject ester is therefore very important.

A fairly recent use of this material is that of a carrier-base in bath oils of the so-called "floating" type, in contradistinction to the older, still popular "dispersible" type, based upon a surfactant in which the perfume oil is optically dissolved.

The perfume oil may constitute as little as 3% of a bath oil, or it may be as high as 50% in certain types of floating bath oils, the balance being mainly the title ester and its homologue (see *iso*-Propyl-palmitate) with smaller amounts of other emollients and perhaps mineral oil.

Prod.: by conventional esterification of *iso*-Propanol with Myristic acid.

106-129; 163-211; 163-235; see also *iso*-Propyl palmitate;

## 2727: n-PROPYL-n-OCT-1-YNE CARBONATE

Propyl octin carbonate.
*n*-Propyl nonynoate.

$CH_3—CH_2—CH_2—OOC—C\equiv C(CH_2)_5CH_3$

$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. B.P. 245° C.

Insoluble in water, soluble in alcohol and oils.

Sweet, intensely green, Violet-leaf type odor of moderate tenacity.

The title ester is very rarely used in perfumery, but it does have some advantage over the conventional acetylenic esters in that it is fresher, sweeter and more "powdery" than most of its relatives.

The ester has found a little use in Cassie, Mimosa, Oriental bases and variations of Violet fragrances, but the latter type perfume is, contrary to repeatedly published "statistical results", certainly not among the most popular fragrance types. It may give very attractive and generally acceptable results as a secondary base.

Prod.: from Methyl-*n*-hexyl ketone to Octyne, then to the acid, from which the *n*-Propylester is prepared by conventional methods.

5-245; 163-66;

## 2728: iso-PROPYL-n-OCT-1-YNE CARBONATE

*iso*-Propyl octincarbonate.
*iso*-Propyl-*n*-nonynoate.

$(CH_3)_2CH{-}OOC{-}C{\equiv}C(CH_2)_5CH_3$

$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. B.P. 236° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, green-leafy, in dilution also fruity, not as sweet as the *n*-Propylester (see previous monograph).

This ester is only very rarely used, and hardly ever offered commercially for use in perfumes. It could be used as a modifier in Violet type fragrances. It does not have the sweet, discretely oily note as found in the *n*-Propylester, and one could be justified in saying that the title material is dispensable. It is practically obsolete in perfumery.

Prod.: from Methyl hexyl ketone via Octyne and its acid to the ester.

5-245;

## 2729: iso-PROPYL PALMITATE

*iso*-Propyl hexadecanoate.
"Deltyl prime" (Givaudan). The title material is main component, while smaller amounts of -laurate and -myristate are present. See also *iso*-Propyl myristate.

$(CH_3)_2CH{-}OOC(CH_2)_{14}CH_3$

$C_{19}H_{38}O_2 = 298.51$

Colorless oily liquid. Sp.Gr. 0.86. M.P. 14°C. Solidifies in the cold.

Practically insoluble in water, soluble in alcohol and oils.

Virtually odorless and tasteless when pure. Commercial grades may occasionally show mildly fatty-oily odor and bland-oily taste, but they should not have any trace of rancid odor. The statement has often been made that the title material "can not become rancid because the chemical does not have any double bonds". The fact remains that certain grades or material from certain suppliers do have an odor which is classified as "rancid" by the perfumer's language. Such off-odor may be due to minute traces of impurities, because any odorous matter will show up very conspicuously in an odorless chemical.

The title ester is not used as an active odorant, fixative or flavor in perfumes or flavor compositions. It is widely employed as a cosmetic emollient, plasticizer and diluent/solvent, often as a major part of the base for the "floating type" bath oil. See also comments made in the monograph: *iso*-Propyl myristate.

Prod.: by esterification of *iso*-Propanol with Palmitic acid. See also monograph: Palmitic acid.

106-130; 163-211;

## 2730: n-PROPYL PELARGONATE

Propyl nonanoate.
Propyl nonylate.

$CH_3(CH_2)_2{-}OOC(CH_2)_7CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless, slightly oily liquid. Sp.Gr. 0.86. B.P. 237° C.

Practically insoluble in water, soluble in alcohol and oils.

Winey-fruity, Melon-like odor with a mildly fermented note and moderate to poor tenacity.

This ester is probably not used in perfume compositions.

Its taste is rather uninteresting, except perhaps as a modifier in Brandy, Melon, Apple and various green-fruity, fresh flavor types. Its contribution to the overall aroma does not justify any extensive experimenting with this ester.

Prod.: by azeotropic esterification of *n*-Propanol with Nonanoic acid.

33-621; 35-514; 103-104; 163-66; 163-235; 163-374;

## 2731: iso-**PROPYL PELARGONATE**

*iso*-Propyl nonanoate.
*iso*-Propyl nonylate.

$(CH_3)_2CH—OOC(CH_2)_7CH_3$

$C_{12}H_{24}O_2 = 200.32$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 228° C.

Practically insoluble in water, soluble in alcohol and oils.

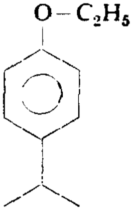
Refreshingly fruity-winey, mildly ethereal-oily odor of moderate to poor tenacity. The fruity notes are rather nondescript, the winey character resembles "fermented" notes.

The title ester has little or no interest to perfumery, but it finds some use in flavor compositions (not listed as G.R.A.S. in the USA) as a modifier in Apple, Coconut, Brandy and various fruit complex flavor types. It is slightly fresher, greener and more ethereal than the *n*-Propylester.

Prod.: by azeotropic esterification of *iso*-Propanol with Nonanoic acid.

## 2732: para-iso-**PROPYL PHENETHOLE**

*para-iso*-Propyl ethoxyphenol.
Australol ethylether.
(*para-n*-Propyl phenethole, which is Homodihydroanethole, is also known, but the author believes that it has no significant use in perfumery).



$C_{11}H_{16}O = 164.25$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet, herbaceous and slightly woody odor of moderate tenacity. Although the sweetness may be classified as "anisic", there is very little resemblance to Anis or Estragon. In fact, the odor is rather chemical and the lack of natural notes makes it difficult to describe the odor of this material properly.

For the same reason probably, this ether has hardly found any sort of application in perfumery. It is rarely offered commercially from the manufacturers of perfume chemicals, and it is absent from most perfume laboratories.

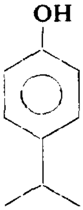
Prod.: by Ethylation of *para-iso*-Propylphenol (= Australol) isolated from Eucalyptus polybractea oil.

The material can also be prepared synthetically from Magnesium *para-iso*-propyl phenylbromide by air oxidation followed by Ethylation with Diethyl sulfate in weak aqueous alkali.

68-421; see also: *para-iso*-Propyl phenol (next monograph).

## 2733: para-iso-**PROPYL PHENOL**

Australol.
*para*-Hydroxycumene.



$C_9H_{12}O = 136.20$

White or colorless, needlelike crystals.
M.P. 62° C. B.P. 229° C.

Slightly soluble in water, soluble in alcohol, oils and aqueous alkali.

Dry-woody, warm, spicy-medicinal odor of moderate to poor tenacity. Less sweet than the Ethyl- and Methyl-derivative (*para*-Cresol), but also less penetratingly medicinal.

The title material has been suggested for use in perfume compositions as a modifier for *para*-Cresol and other phenols. However, it lacks the ability to perform with any sort of floral note, such as obtained with *para*-Cresol. Accordingly, the use of the title material becomes very limited, and it is reasonably fair to say that the title phenol is dispensable in perfumery.

Prod.:

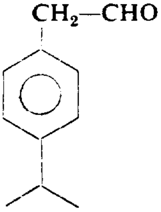
1) by isolation from Eucalyptus polybractea oil.
2) from Magnesium *para-iso*-propylphenylbromide by air oxidation.

68-421; 90-388; 160-1158; 163-40; 163-211; B-VI-505;

## **2734:** para-iso-**PROPYL PHENYLACETALDEHYDE**

"Cortexal".
Homo-cuminic aldehyde.
Cymyl acetaldehyde (older name).
Cumyl acetaldehyde.
Cuminic acetaldehyde.
*4-iso*-Propyl phenylacetaldehyde.
*para*-Cymene-7-carboxaldehyde.

The perfumery literature is particularly inconsistent with respect to the nomenclature of the title chemical. Confusion goes so far, that odor descriptions can be totally misleading.



$C_{11}H_{14}O = 162.23$

Colorless liquid. Sp.Gr. 0.97. B.P. 243° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, green, refreshingly bark-woody or sap-like odor of moderate to good tenacity.

In concentrations of less than 10 ppm the flavor is citrusy, remotely Orange-like, rather bitter-sweet, fruity. At higher concentrations it is not quite pleasant, bitter, pungent, green.

The odor is sometimes described as Orange-Verbena-like, but few perfumers seem to underwrite such odor description if the material is submitted "on a blind test" (no name given).

This aldehyde has been marketed for many years under a trade name and is now also available under its proper chemical name. It is used in modern perfumes to create new and attractive topnotes in combination with Oakmoss, Citrus oils, alifatic aldehydes, etc. and it is particularly suitable in non-floral fragrance types. It performs excellently where Vetiver, Styrax, Sandalwood, Ionones, Galbanum, etc. are used, and its tenacity will carry it into the heart of the fragrance if it is introduced in proper balance. For special effects, such as "wet bark", fresh, green flower stalks, Chrysanthemum bouquets, etc. it may form a major part of the fresh, natural-green complex. With Bitter Orange or Grapefruit oil, it will produce new and very pleasant notes and interesting variations from the very conventional Citrus topnote complex.

The title aldehyde is also used in flavor compositions for fruit complexes, Lemon, Orange, Arak, etc. It was once used in combination with Coumarin to imitate the aroma of the Woodruff (Asperula odorata), also used in the flavoring of the German specialty "May Wine".

The concentration of this aldehyde in finished products may be as low as 0.1 to 1 ppm.

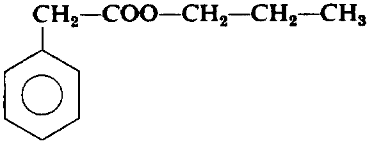
G.R.A.S. F.E.M.A. No.2954.

Prod.: from Cumyl Magnesiumchloride plus Ethyl formate or Triethyl *ortho*-formate, followed by acid hydrolysis of the acetal.

7-224; 36-1027; 102-53; 103-254; 103-287; 59-59; 103-296; 163-40; 163-350; B-VII-262;

## 2735: n-PROPYL PHENYLACETATE

*n*-Propyl-*alpha*-toluate.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Sp.Gr. 0.98. B.P. 253° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Honey-like, but fresh and light, fruity Apricot-Rose type odor of moderate tenacity.

Powerful, fruity-rosy, honeylike taste in concentrations lower than 10 ppm. The honeylike, rosy character is perceptible far below 1 ppm.

This ester is used in perfume compositions for Lilac, Rose (type tearose), Lily, Hyacinth, Honey and wax odors, etc.

Its power is often underestimated, and it will often be necessary to study the fragrance for several weeks to make certain that the ester does not "stand out". It is less versatile and more difficult to handle than the *iso*-Butylester, which is probably the most interesting of all the Phenylacetates. Its low cost and ready availability makes it quite popular, and it is often used in "Oriental" type soap and detergent fragrances.

The subject material is furthermore used in flavor compositions for its powerful effect in imitation Apricot, Grenadine, Peach, Date, Fig, Honey, Blackcurrant, etc. and in Tobacco flavorings. Traces are used in certain types of Butter and Caramel flavor, and the ester is often used in Rose type of beverage flavor.

The concentration used is normally as low as 0.5 to 5 ppm in the finished product.

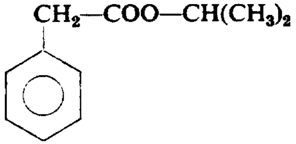
G.R.A.S. F.E.M.A. No.2955.

Prod.: by azeotropic esterification of *n*-Propanol with Phenylacetic acid.

33-621; 163-66; 163-374;

## 2736: iso-PROPYL PHENYLACETATE

*iso*-Propyl-*alpha*-toluate.



$C_{11}H_{14}O_2 = 178.23$

Colorless liquid. Sp.Gr. 0.99. B.P. 238° C.

Almost insoluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful, ethereal or winey-honey-like, sweet odor of moderate tenacity. Fresher than the odor of the *n*-Propylester, but not quite as sweet. The odor has often been described as resembling that of dry leaves, but the author finds it difficult to underwrite this description. However, in extreme dilution, the material has a vague odor resemblance to tea and this could have been the base for the above odor description.

The title ester has found some use in perfume compositions, partly in heavy-sweet florals (Honeysuckle and tropical flower types), partly as ingredient of winey or honeylike bases. The preferred ester is, however, the *iso*-Butyl phenylacetate with its unsurpassed versatility, low cost and good stability.

This ester is also used in imitation Butter, Caramel, Honey and a few other types of flavor. The concentration in the finished product is normally about 0.5 to 10 ppm.

G.R.A.S. F.E.M.A. No.2956.

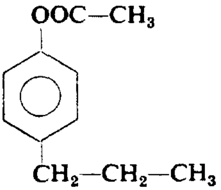
Prod.: by azeotropic esterification of *iso*-Propanol with Phenylacetic acid.

The ester has also been produced by acid hydrolysis of Benzyl cyanide in *iso*-Propanol solution.

32-245; 163-40; 163-66;

## 2737: para-n-**PROPYL PHENYL ACETATE**

*para-n*-Propyl-*1*-acetylphenol.



$C_{11}H_{14}O_2 = 178.23$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Weak and uninteresting, anisic-sweet, but also harsh odor of moderate tenacity.

This isomer of the Propyl phenylacetates is briefly mentioned in this work since it has been confused with the two more useful esters of Phenylacetic acid.

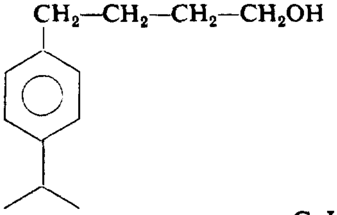
The title material has very little, if any, interest to the perfumer or the flavorist.

Prod.: by Acetylation of *para-n*-Propyl phenol (Dihydro chavicol).

68-421; 31-125;

## 2738: para-iso-**PROPYL PHENYLBUTANOL**

*para-iso*-Propyl phenylbutylalcohol.
4-(*para-iso*-Propylphenyl)-butanol-*1*.
4-Cumenylbutanol-*1*.



$C_{13}H_{20}O = 192.30$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Mildly green, woody-floral odor of moderate tenacity. The woody notes tend to become herbaceous upon dilution, and the green notes are rather sweet, not pungent.

This alcohol has been suggested for use in perfume compositions, but it is very rarely, if ever, offered commercially under its proper chemical name.

It could find use in Mimosa, Lilac, Oriental, Chypre, etc. since it blends excellently with the Ionones, Methylionones, Cinnamic and Anisic alcohol and esters, Oakmoss, newer Cyclohexanol derivatives, etc.

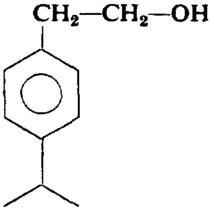
Although the chemical has been known for quite a number of years, it has failed to become widely known, and one may assume that this is a sign of its passing into oblivion gradually.

Prod.:

1) from *para*-Cumenyl ethylmagnesiumbromide plus Ethylene oxide.
2) from Homocuminic aldehyde plus Acetaldehyde by condensation, followed by hydrogenation and reduction.

## 2739: beta-para-iso-**PROPYL PHENYLETHYL ALCOHOL**

*beta-para*-Cymyl ethanol.
Homocuminic alcohol.
Cuminyl carbinol.



$C_{11}H_{16}O = 164.25$

Colorless liquid. B.P. 258° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, mildly oily-floral odor of good tenacity.

The title alcohol has been suggested for use in perfume compositions as a modifier/blender with fixative effect. It blends particularly well with the Methylionones, Bergamot, Lavender, Lavandin, Mimosa and Orris bases, Oakmoss and Galbanum, etc.

The material has occasionally been used in Chypre, Oriental Balsamic-woody and herbaceous fragrance types, but it is rarely offered commercially under its proper chemical name.

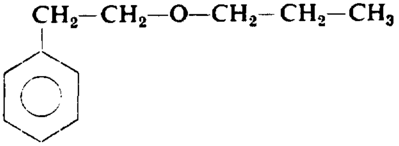
Prod.:

1) by hydrogenation of *para-iso*-Propyl cyclohexane ethanol.
2) by reduction of Homocuminic aldehyde – see monograph: *para-iso*-Propyl phenylacetaldehyde.

163-350;

## 2740: PROPYL PHENYLETHYL ETHER

Phenylethyl propyl ether.



$C_{11}H_{16}O = 164.25$

Colorless mobile liquid. B.P. 227° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, earthy-floral, deep and warm odor of poor tenacity, but considerable diffusive power.

This ether has found a little use in perfume compositions as a modifier for its lower homologues, both of which are rather pungent and at times difficult to control in a perfume creation. They demand very skilful fixation, while the title ether is more subdued, not as agressive in its pungent floral notes.

The title ether blends well with Coumarin and Amylsalicylate in novel types of Fougère, and it gives interesting variations to a Lavender if the perfumer plays on the earthy notes in the ether to support the herbaceous-earthy portion of Lavender (or Geranium, too).

The subject ether can give power to various heavy floral fragrance types, exotic flower bases, Oriental-balsamic fragrances, in which Opopanax may be a significant component, etc.

Prod.:

1) from Phenylethyl magnesium chloride plus Bromodiethylether.
2) from Phenylpropionic aldehyde dimethylacetal by reduction in presence of a Nickel catalyst at 180° C.

163-63;

See also monographs:

Ethyl phenylethyl ether (1338),

Methyl phenylethyl ether (2192),

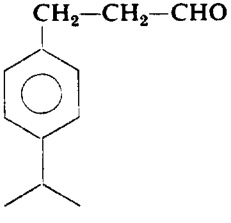
Phenylethyl vinyl ether (2559).

## 2741: 3-(para-iso-PROPYLPHENYL)-PROPIONIC ALDEHYDE

*3(para-iso*-Propylphenyl)-propanal-*1*.

*para-iso*-Propyl hydrocinnamic aldehyde.

*para*-Cymyl propanal.



$C_{12}H_{16}O = 176.26$

Colorless, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, sweet-green, refreshingly light, floral odor of good tenacity.

Peculiar, sweet-green, fresh-fruity flavor at concentrations lower than 10 ppm. Rather perfumey, unnatural at higher levels.

This aldehyde is occasionally used in perfume compositions as a floralizer in Muguet bases, or as a part of the floral-green theme of various delicate floral fragrance types.

It is more commonly used in flavor compositions, e.g. as a power factor in fruit complexes, a special note to introduce fresh or green nuances, sometimes also classified as an aroma floralizer. Its presence may distract the human taste sensation from rough or weedy-fresh notes derived from topnotes or volatile substances in essential oils, etc. and the title aldehyde actually "rounds-off" the flavor.

Prod.:

1) by condensation of Cumin aldehyde with Acetaldehyde, followed by hydrogenation to the saturated aldehyde.
2) from Cumyl magnesium chloride and Propylformate, followed by acid hydrolysis of the resulting acetal.

G.R.A.S. F.E.M.A. No.2957.

163-211; See also 2717.

## 2742: n-PROPYL PROPIONATE

Propyl propanoate.

$CH_3—CH_2—CH_2—OOC—CH_2—CH_3$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.88.
B.P. 123° C.

0.5% soluble in water, miscible with Propylene glycol, alcohol and oils.

Fresh-ethereal, fruity-floral odor of very poor tenacity. The fruity notes being Apple-Pineapple-like, while the floral character is more of a general "lift" of sweetness.

The title ester finds very little use in perfumery in spite of the fact that it could introduce very attractive "lift" in topnote compositions for floral and Citrus-type bases, etc.

It is frequently used in flavor compositions for imitation Apple, Banana, Cherry, Melon, Peach, Plum, and in "tutti-frutti", Rum flavors, Pineapple, etc.

The concentration is normally about 5 to 30 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2958.

Prod.: by azeotropic esterification of *n*-Propanol with Propionic acid.

26-666; 33-620; 100-864; 103-104; 160-1188; 163-66; 163-374; B-II-240;

## 2743: iso-PROPYL PROPIONATE

*iso*-Propyl propanoate.

$(CH_3)_2CH—OOC—CH_2—CH_3$

$C_6H_{12}O_2 = 116.16$

Colorless mobile liquid. Sp.Gr. 0.89.
B.P. 111° C.

0.5% soluble in water, miscible with alcohol, Propylene glycol and oils.

Fresh-ethereal, fruity odor with fermented-winey note and poor tenacity. Fruity, Rum-like taste in concentrations lower than 100 ppm. This ester is probably not used in perfumes.

It finds some use in flavor compositions, mainly in fruit complexes, "tutti-frutti"-types, Rum imitation, etc. It produces great "lift" to the flavor and is quite compatible with most fruit flavors.

The concentration used is about 10 to 50 ppm in the finished product.

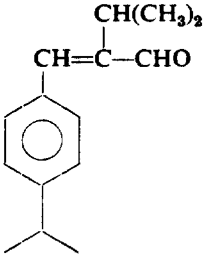
G.R.A.S. F.E.M.A. No.2959.

Prod.: by azeotropic esterification of *iso*-Propanol with Propionic acid.

7-224; 26-666; 140-137; B-II-241;

## 2744: alpha-iso-PROPYL-para-iso-PROPYL CINNAMIC ALDEHYDE

*3-(para-iso-*Propylphenyl)-*2-iso-*propyl-*2-*propen-*1*-al.



$C_{15}H_{20}O = 216.33$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Peculiar, semi-dry, leafy-floral odor of considerable depth and tenacity.

The material is very rarely offered commercially (under its proper chemical name) and the author has doubts about the olfactory quality of the samples received. The title material is notoriously problematic to produce in consistent olfactory quality, and this may be one reason for its absence from the market.

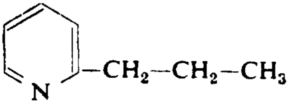
This aldehyde could possibly find use in perfumes as a modifier for Cyclamen aldehyde and its homologues, although a certain roughness seems to be normal in the types with unsaturated chain (as the title material), while the more successful types have a saturated side chain. However, experience with Amylcinnamic aldehyde seems to show the opposite effect, and there is no proof that the key to a successful type is to be found in one or the other chemical group of these aldehydes.

Meanwhile, the title material remains hidden in the overpopulated shelves in the research files, probably not in the perfumer's laboratory.

Prod.: by condensation of Cuminaldehyde with *iso*-Valeric aldehyde.

## 2745: 2-n-PROPYL PYRIDINE

*alpha-n-*Propyl pyridine.
Conyrine.



$C_8H_{11}N = 121.18$

Almost colorless or very pale straw-colored oily liquid. Sp.Gr. 0.92. B.P. 159° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, sweet and, when undiluted, nauseating odor. In dilution green-anisic, slightly minty and tobacco-like, exotic-heavy, with moderate tenacity. Some authors report a floral odor in this material. Typical for the alkylpyridines is the strong effect of impurities upon the terminal notes. A highly purified material will usually fade away on a perfume blotter with gradually decreasing power of the initial odor type, while impure material will show an increasingly conspicuous, new odor type, usually less attractive, less desirable.

This Pyridine has been suggested for use in perfume compositions, and it is definitely one of the few to be taken into consideration for experimental fragrance creation. Traces of this material may introduce very natural, green-tobacco-like, herbaceous notes in a Fougère or Chypre, particularly in conjunction with Oakmoss, Lavender, Phenylacetates, etc.

Prod.:

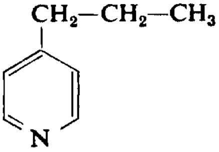
1) by Wolff-Kishner reduction of Propionyl pyridine. This process yields exclusively the *alpha*-isomer (if intermediate *alpha*- was used).
2) from Pyridine and *n*-Propylbromide. This process yields a mixture of *alpha*- and *gamma*-isomers, see next monograph.

69-524; 159-432; 100-282; B-XX-247;
Sample: Reilly Tar & Chemical Corp., Indianapolis, USA.

NOTE: The completely hydrogenated derivative *alpha*-Propyl-piperidine, is known better under the name Coniine. It is one of the most powerful poisons (alkaloids) known. The lethal dose for a human being is about 0.10 to 0.12 grams. Doses of 0.03 grams are considered hazardous.

## 2746: gamma-n-**PROPYL PYRIDINE**

*4-n*-Propyl pyridine.



$C_8H_{11}N = 121.18$

Pale straw-colored or almost colorless oily liquid. Sp.Gr. 0.93. B.P. 184° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, sweet-nauseating, but in dilution heavy-herbaceous odor. Overall less minty, less sweet, and more heavy-pungent-herbaceous than the *alpha*-isomer (see previous monograph).

Some authors report a Violet type odor in this material.

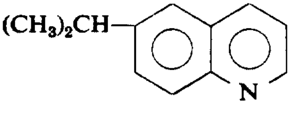
This Pyridine has been suggested for use in perfume compositions, but the author is inclined to recommend experimentation with the *alpha*-isomer, and not with the title material. It has very little to offer of interest to the perfumer, unless a highly purified material should prove to be much more attractive than the commercially available grade, which is originally intended for the chemical industry as an intermediate for synthesis, not as a perfume chemical to be used as such.

Prod.: by Wolff-Kishner reduction of *gamma*-Propionyl pyridine. It has also been prepared from Pyridine and *n*-Propylbromide, but this method yields a mixture of *alpha*- and *gamma*-isomers.

30-266; 69-524; 159-432; B-XX-248;

## 2747: 6-iso-**PROPYL QUINOLINE**

*para-iso*-Propyl quinoline.
"Lichenol" (confusing, this name is also used for Methyl everninate).
The title material is often called:
*iso*-Propylquinoline.



$C_{12}H_{13}N = 171.24$

Pale yellowish or pale amber-colored or almost colorless oily liquid. Sp.Gr. 1.03. B.P. 260° C.

Slightly soluble in water, soluble in alcohol and oils, also soluble in dilute mineral acids.

Powerful and diffusive, yet very tenacious earthy-woody, root-like odor. Upon dilution, the odor becomes more spicy-earthy, warm, but still sharp.

This material is one of the more popular Quinolines. It is frequently used as a trace additive to woody fragrances, including Methylionones and Vetiver products, Cedarwood-derivatives, etc. It will also enhance floral notes, but not with the same attractive effect as noticed with *iso*-Butyl quinoline (see monograph).

The title material is furthermore used in artificial Vetiver oil (Vetiver "extender") and in Oakmoss bases, Reseda compositions, etc. and in general to enhance mossy notes in Chypre, Oriental, Fougère and many other fragrance types.

A number of other isomers are known, but they seem to have lost their initial popularity, leaving the "*para-*" as the only common derivative found in the perfume laboratory. The *2-* and the *8-iso-*Propyl quinoline were used several decades ago, but the author believes that they can be considered as obsolete in Perfumery.

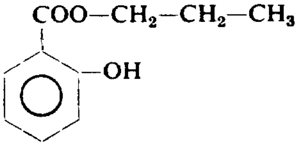
Prod.:

1) by Skraup's reaction from *para-iso-*Propylaniline plus Acrolein.
2) from Quinoline hydrochloride plus Propylene at high temperature and pressure over an Aluminum silica type catalyst.

4-70; 7-225; 7-252; 7-352; 86-75; 106-210; 156-319; 163-40; 163-211;

## 2748: n-PROPYL SALICYLATE

*n-*Propyl-*ortho-*hydroxybenzoate.



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid. Sp.Gr. 1.09.
B.P. 255° C.

Very slightly soluble in water, miscible with alcohol and oils.

Fruity-herbaceous, sweet Clover-like, Plum-like odor with a winey note and good tenacity.

The title ester represents the transition stage of Salicylates from the very sweet, fruity-Wintergreen like character to the very heavy herbaceous-floral type as found in Amylsalicylate and higher esters.

This particular odor is not very much in demand, and has never attracted the perfumer. It is not typically fruity enough to attract the interest of the flavorist.

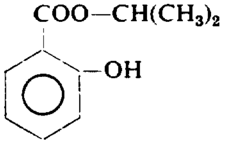
Accordingly, the ester finds only little use in perfume compositions as a modifier in Fougères, where the odor is very compatible. The ester is inexpensive and relatively stable, but offers the same disadvantages as many other Salicylates, in color reactions due to its phenolic Nature.

Prod.: by azeotropic esterification of *n-*Propanol with Salicylic acid.

26-666; 33-621; 34-788; 163-66; 163-235; B-X-75;

## 2749: iso-PROPYL SALICYLATE

*iso-*Propyl-*ortho-*hydroxybenzoate.



$C_{10}H_{12}O_3 = 180.21$

Colorless oily liquid. Sp.Gr. 1.08.
B.P. 240° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-ethereal-herbaceous, yet quite tenacious odor with distinctly fruity character.

This ester is often sold under the name "Propyl salicylate", but it is in very weak demand and probably less desirable than the *n-*Propylester (see previous monograph).

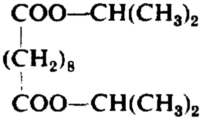
It finds a little use in Fougère and Clover perfumes, as well as in various low-cost fragrances for household products, detergents, etc.

Prod.: by azeotropic esterification of *iso-*Propanol with Salicylic acid.

26-666;

## 2750: iso-PROPYL SEBACINATE

Di-*iso*-propyl sebacate.
Di-*iso*-propyl decane dioate.



$$\begin{array}{l} \mathrm{COO{-}CH(CH_3)_2} \\ | \\ \mathrm{(CH_2)_8} \\ | \\ \mathrm{COO{-}CH(CH_3)_2} \end{array}$$

$C_{16}H_{30}O_4 = 286.42$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very mild, sweet-oily-ethereal odor and bland-sweet, mildly fruity taste in concentrations near 100 ppm. Practically tasteless at lower levels of concentration.

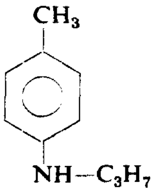
This ester is sometimes used in perfume compositions as a blender/solvent or sweetener/diluent. Mostly in low-cost perfumes, or in compositions where the total cost has to be adjusted for some very strong reason. The material does not depress the overall odor quite as much as noticed with Diethyl phthalate, but there may be a slight addition of ethereal odor with the use of the title ester in higher concentrations.

Prod.: by azeotropic esterification of *iso*-Propanol with Sebacic acid.

163-66;

## 2751: n-PROPYL-para-TOLUIDINE

*1*-Methyl-*4*-*n*-propylaminobenzene.
The commercial grade material will often contain perceptible amounts of *n*-Propyl-*ortho*-Toluidine.



$C_{10}H_{15}N = 149.24$

Colorless oily liquid. B.P. 251° C.

Acquires a brownish-reddish color when exposed to air and daylight.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-animal-floral odor with heavy-mossy character and good tenacity. Pungent when undiluted, heavy-floral in dilution.

This material is rarely offered commercially but it has been used from time to time as a trace ingredient in Oriental-floral or woody mossy fragrance types. It performs very well with the Quinolines, Phenylacetates, etc. and it gives attractive sweet background for a Lilac fragrance.

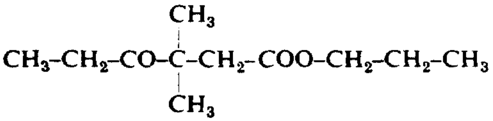
Although Alkyl-anilines and Alkyl-aryl anilines are considered much less toxic and generally less hazardous than Aniline, one should always keep the possible hazard in mind if these materials go beyond experimental use into functional (consumer) products.

Prod.: from Propanol and *para*-Toluidine in vapor phase over Aluminum oxide at 400-420° C.

68-171;

## 2752: n-PROPYL-2,2,4-TRIMETHYL-3-OXOVALERATE

*2,2,4*-Trimethyl-*gamma*-ketovaleric acid, *n*-Propylester.
"*iso*-Hexyl levulinate".
*n*-Propyl-*2,2,4*-trimethyl-levulinate.



$$\mathrm{CH_3{-}CH_2{-}CO{-}}\overset{\overset{\mathrm{CH_3}}{|}}{\underset{\underset{\mathrm{CH_3}}{|}}{\mathrm{C}}}\mathrm{{-}CH_2{-}COO{-}CH_2{-}CH_2{-}CH_3}$$

$C_{11}H_{20}O_3 = 200.28$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, slightly winey-sweet, moderately tenacious odor.

This rare ester has been suggested for use in certain artificial essential oils, and as a novel note in warm-herbaceous bases, in support of Chamomile, Clary Sage, Lavender, etc. for Chypre and modern herbaceous-fruity fragrance types, etc.

The material is rarely offered under its proper chemical name, but it is generally prepared by the interested company for use in bases.

Although there is no apparent indication that the material is used in flavor compositions, the author finds it quite possible that it could eventually be used as a bouquetting material in Butterscotch, Caramel, Rum, fruit complexes, Plum, etc.

The ketoester is not included in the American G.R.A.S. list.

Prod.: from *asymmetric*-Dimethyl succinyl chloride plus Zinc ethyl, followed by esterification of the resulting acid with *n*-Propanol. Other methods are known.

66-882;

## 2753: 1-PROPYL TRISULFIDE

Dipropyl trisulfide.

$CH_3–CH_2–CH_2–S–S–S–CH_2–CH_2–CH_3$

$C_6H_{14}S_3 = 182.38$

Almost colorless or pale yellowish mobile liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very powerful and diffusive, Garlic-like odor, penetrating and repulsive when undiluted, but in extreme dilution rather pleasant, sweet-herbaceous, distinctly Garlic-like.

The flavor of this material is almost exclusively based upon its odor, since the material is not a lachrymator.

After being identified in Onion volatile oil, this Trisulfide has been synthesized and is used in the flavoring of Onion and Garlic products, reconstitution of flavor in dried Onion or Garlic, in meat sauces and dressings, etc.

It constitutes a minor part of the entire flavor and does not have the pungency of Onion.

158-136; 157-391;

## 2754: PROPYL UNDECYLATE

*n*-Propyl undecanoate.

$CH_3—CH_2—CH_2—OOC(CH_2)_9CH_3$

$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid. Sp.Gr. 0.85.
B.P. 250° C.

Insoluble in water, soluble in alcohol and oils.

Lemon-citrusy, oily-winey, mild odor of good tenacity.

Mild, citrusy-oily taste in concentrations below 10 ppm. The minimum perceptible is quite low, in spite of the fact that the material can not be classified as a powerful aroma.

The ester has very little use in perfumery, except for occasional application in Cognac bases or Citrus complex topnote compositions, etc.

It is used in flavor compositions for imitation green Grape and sometimes also for Grapefruit. However, the ester is not specifically mentioned in the American G.R.A.S. list.

Prod.: by azeotropic esterification of *n*-Propanol with Undecanoic acid.

35-851; 163-235;

## 2755: n-PROPYL UNDECYLENATE

*n*-Propyl undecenoate.

$CH_3—CH_2—CH_2—OOC(CH_2)_8CH{=}CH_2$

$C_{14}H_{26}O_2 = 226.36$

Colorless oily liquid. Sp.Gr. 0.88.
B.P. 268° C.

Practically insoluble in water, soluble in alcohol and oils.

Heavy-fruity-oily odor of moderate to good tenacity. Less vinous than the saturated ester (see previous monograph), yet still reminiscent of Brandy (odor of "empty Brandy bottle").

The title ester finds probably very little use in perfumes, except as a trace ingredient in Gardenia and a few other heavy florals. It is occasionally used in flavor compositions, mainly imitation Rum, Peach, Mango and various fruit complexes or wine flavors.

The ester is not listed in the American G.R.A.S. list.

Prod.: by azeotropic esterification of *n*-Propanol with Undecylenic acid.

163-66; 3-108;

## 2756: iso-PROPYL UNDECYLENATE

*iso*-Propyl undecenoate.

$(CH_3)_2CH—OOC(CH_2)_8CH{=}CH_2$

$C_{14}H_{26}O_2 = 226.36$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 260° C.

Practically insoluble in water, soluble in alcohol and oils.

Citrusy, oily-Orange-like, winey and Brandy-type odor of moderate to good tenacity.

Sweet and mild, fruity-Brandy-like taste in concentrations below 10 ppm.

This ester finds only very little use in perfumes.

It is occasionally used in flavor compositions for imitation Apricot, Rum, Brandy, in Citrus complexes, etc.

The subject ester is not listed in the American G.R.A.S. list.

Prod.: by azeotropic esterification of *iso*-Propanol with Undecylenic acid.

35-854; 163-66; 163-211; 3-108;

## 2757: n-PROPYL-n-VALERATE

*n*-Propyl-*n*-pentanoate.
Propyl valerianate.

$CH_3—CH_2—CH_2—OOC(CH_2)_3CH_3$

$C_8H_{16}O_2 = 144.21$

Colorless mobile liquid. Sp.Gr. 0.87.
B.P. 167° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Powerful and relatively diffusive, fruity-ethereal, Apple-like and also Pineapple-like odor of poor tenacity.

Sweet-fruity, ethereal, Apple-and-wine-like taste in concentrations below 50 ppm.

This ester finds very little use in perfumes, but it is used occasionally in flavor compositions, mainly those of Apple-like, fruity-wine-like and fruit-complex type. Its flavor effect is not quite as Pineapple-like as that of the *iso*-Propylvalerate.

The material is not listed in the American G.R.A.S. list, but the two *iso*-Valerates are included in that list.

Prod.: by azeotropic esterification of *n*-Propanol with *n*-Valeric acid.

33-621; 33-933; 163-66; 163-235; B-II-301;

## 2758: n-PROPYL-iso-VALERATE

*n*-Propyl-*beta*-methylbutyrate.

$CH_3—CH_2—CH_2—OOC—CH_2—CH(CH_3)_2$

$C_8H_{16}O_2 = 144.21$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 156° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Light, powerful, slightly winey, fruity Apple-Pineapple type odor of poor tenacity. Fresher and more Pineapple-like than the *n*-Propyl-*n*-valerate.

Sweet-ethereal-fruity, Apple-Pineapple-like taste in concentrations lower than 50 ppm.

The title ester has little or no application in perfumes, except in rare cases where it forms part of topnote composition for exotic floral bases. It is used quite frequently in flavor compositions, mainly in imitation Apple, Banana, Peach, Pineapple, Strawberry, etc. Concentrations are about 5 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2960.

Prod.: by azeotropic esterification of *n*-Propanol with *iso*-Valeric acid.

33-932; 163-235; B-II-312;

## 2759: iso-PROPYL-n-VALERATE

*iso*-Propyl-*n*-pentanoate.
*iso*-Propyl valerianate.

$(CH_3)_2CH—OOC—CH_2—CH_2—CH_2—CH_3$

$C_8H_{16}O_2 = 144.21$

Colorless mobile liquid.

Very slightly soluble in water, soluble in alcohol, Propylene glycol, Glycerin and oils.

Diffusive, ethereal-fruity, winey odor of Apple-Brandy-like character and poor tenacity.

The title ester is rarely, if ever, used in perfumes. It does not seem to occur much in flavors either, but the author has decided to include the material in this work for the sake of completing the monographs on the four Propylvalerates. This is the least interesting of the four isomer esters.

## 2760: iso-PROPYL-iso-VALERATE

*iso*-Propyl-*iso*-pentanoate.
*iso*-Propyl-*beta*-methylbutyrate.
*iso*-Propyl-*iso*-valerianate.

$(CH_3)_2CH—OOC—CH_2—CH(CH_3)_2$

$C_8H_{16}O_2 = 144.21$

Colorless mobile liquid. Sp.Gr. 0.85.
B.P. 145° C.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Ethereal-fruity, diffusive and winey, Pineapple-type odor of poor tenacity.

Sweet-fruity, Pineapple-like taste in concentrations below 50 ppm.

The title ester is rarely used in perfumes. Traces may be used as part of topnote compositions for floral bases.

It finds some use in imitation Pineapple, and as refreshing note in Nut flavors, where most of the active ingredients have rather heavy aroma. It brings a pleasant lift to such flavor types, and its fruity contribution may be kept at a minimum by proper dosage.

Concentrations of this ester in consumer products are usually about 5 to 15 ppm.

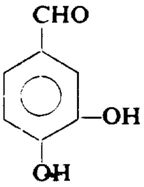
G.R.A.S. F.E.M.A. No.2961.

Prod.: by azeotropic esterification of *iso*-Propanol with *iso*-Valeric acid.

163-40; B-II-312;

## 2761: PROTOCATECHU ALDEHYDE

Protocatechuic aldehyde.
*3,4*-Dioxybenzaldehyde.
*3,4*-Dihydroxy benzaldehyde.



$C_7H_6O_3 = 138.13$

White or colorless plate-like crystals.
M.P. 153° C under decomposition.

5% soluble in cold water, 33% soluble in boiling water. Soluble in alcohol and aqueous alkali, also in some, but not all, perfume oils.

This material has only a faint odor, normally not pleasant, rather medicinal, dry and weak.

The title aldehyde is included in this work mainly to supply a further background for the monographs of many perfume and flavor materials, derived directly or indirectly from this aldehyde. It has also been the target of some olfactory and organoleptic studies, since certain theories claim that the substitution in positions 1, 3 and 4 is one of the favorable combinations of radicle substitution on the benzene ring as far as sweetness and aromatic power is concerned. But further studies aim at determining what type of radicles are needed, and exactly where.

Apparently, the presence of two hydroxyl (phenol) groups have a distinctly depressing effect upon the powerful odorant, Benzaldehyde. Yet, aromatic power and sweetness is restored when one phenolgroup is alkylated to form an ether (e.g. Vanillin). Even the simpler *para*-Hydroxy benzaldehyde is practically odorless, while its Methylether (Anisaldehyde) is a powerful odorant. The reader is referred to special literature on this subject. Many books deal exclusively with such studies, philosophy and tentative conclusions.

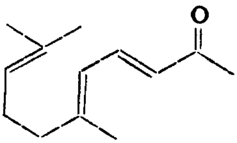
The title material can be produced in many ways, e.g.:

1) from Catechol (Pyrocatechin) by Reimer-Tiemann reaction (treatment with Chloroform and Potassium hydroxide).
2) from Vanillin by De-methylation.
3) from Heliotropine with Aluminum chloride.
4) from Veratraldehyde.

61-61; 68-746; 90-526; 100-866; 95-144; 96-134; B-VIII-246;

## 2762: PSEUDO IONONE

Citrylidene acetone.
*2,6*-Dimethylundeca-*2,6,8*-trien-*10*-one.
The commercial product will usually be a mixture of two diastereoisomeric materials.



$C_{13}H_{20}O = 192.32$

Pale yellowish oily liquid. Sp.Gr. 0.89.
B.P. 258° C.

Practically insoluble in water, soluble in alcohol and oils.

Oily-balsamic, warm-floral odor of Jasmin-Violet character and good tenacity. The odor is overall harsher than that of the Ionones, but the floral character seems more versatile. There is a common mistake in judging the Pseudo ionones from the very impure grades often available as "redistilled tail fractions" from the Ionone distillation (Pseudo ionone is higher boiling than Ionone).

A purified, intentionally produced Pseudo ionone has a relatively pleasant odor. Its Dihydro-, Tetrahydro- and particularly its Hexahydro-derivative have acquired considerable interest and success in perfumery.

Pseudo ionone is sometimes used in perfume compositions for its mellowing, sweet-woody-balsamic effect in Jasmin variations, in Violet bases and in certain types of Oriental fragrance.

Prod.: by condensation of Acetone with Citral. This is the first step in the conventional method of manufacturing Ionones. These ketones are produced by cyclization of Pseudo ionone.

5-170; 31-95; 95-166; 96-167; 156-200; 163-67; 163-236; 163-374;
See also: 1432-1588-2925.

## 2763: PSEUDO LINALYL ACETATE

Not a well-defined, single chemical.

The commercial product, known under the title name (I.F.&F.) or as "Neobergamate" (Naarden, N.V.), is a mixture of a great number of esters, alcohols and terpenes, with Myrcenyl acetate as chief component. It constitutes approximately one-third of the commercial material.

Pseudo linalylacetate was manufactured almost ten years before Myrcenyl acetate as such became a commercial article. The title material was intended to be a powerful, sweet-spicy, warm-citrusy odorant, stable in soap, and compatible with the conventional soap and detergent perfume materials.

In spite of a cost which for the last 7 years has been far in excess of the price of Linalyl acetate (synthetic), it was very successful and effective for its purpose. In soap, it is far superior to Linalyl acetate in power, radiation and stability.

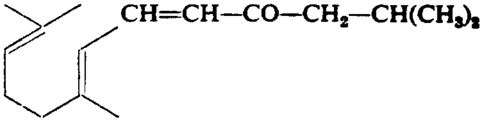
As component of artificial Bergamot, Lavender and Nutmeg – not the "reconstituted types" – the title material has also found considerable interest.

Prod.: by treatment of Myrcene with Acetic acid and Sulfuric acid at controlled temperature. The conditions of temperature, acidity, etc. largely monitor the composition of the resulting product, which is composed of selected fractions from the vacuumdistilled reaction mixture. Presumably more than 30 components contribute to the odor of the title material.

163-236;
See also 156-374; and monograph: Myrcenyl acetate.

## 2764: PSEUDO METHYL ETHYL IONONE

*2,6,12*-Trimethyl-trideca-*2,6,8*-trien-*10*-one.
Citrylidene (methyl)-*iso*-butyl ketone.



$C_{16}H_{26}O = 234.38$

Pale straw-colored, oily liquid. B.P. 280° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and very tenacious, floral-woody and powdery odor. The pure material is not a commercial article, but the ketone occurs as a component of various perfume specialties.

The title ketone has an enhancing effect upon the odor of the desirable and more common types of Methylionone and their higher homologues. Since the material represents an intermediate in the manufacture of one such higher homologue, it has been known for quite some time, and its presence in the Ionone homologue has been thoroughly studied. Contrary to statements made from time to time, many of the Pseudo ionones have quite attractive odors, in fact it was stated as early as in 1892 by some of the originators of the Ionones, that Pseudo ionone, when purified, has a very attractive odor, later claimed to be superior to that of Ionone (German patent for Pseudo ionone, dated 1899).

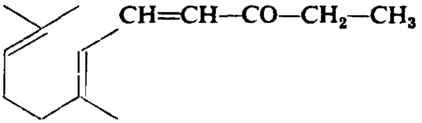
The subject material is used indirectly (as part of a specialty) in finer perfumes, where certain Methylionone types are employed at relatively high concentration. With refined Vetiver products, Oakmoss extracts, and discrete floral materials, it can produce very popular "powdery" dry-sweet notes of outstanding tenacity. This type of odor may be the base for a luxury perfume.

Prod.: by condensation of Citral with Methyl-*iso*-butylketone. The process leads to Methyl ethyl ionones after cyclization of the (title) condensation product.

163-374;
See also monograph: Methyl ethyl ionone (*alpha*-) (766).

## 2765: PSEUDO METHYL IONONE

Pseudo-*normal*-methyl ionone.
Citrylidene (methyl) ethyl ketone.
*2,6*-Dimethyldodeca-*2,6,8*-trien-*10*-one.
The material exists in *cis*- and *trans*-forms.



$C_{14}H_{22}O = 206.33$

Pale straw-colored oily liquid. Sp.Gr. 0.89. B.P. 271° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, oily-woody, discretely floral odor of good tenacity. The odor is heavily influenced by the presence (or absence) of trace amounts of Methylionones or other (lower boiling) related materials. The Pseudo-methylionones resulting from a process aimed at making just Pseudo methylionones will usually have an odor much superior to the odor of Pseudomethylionones resulting from a fractionated distillation of Methylionones *after* the cyclization process.

The title ketone and its isomer (see next monograph) serve as additives to perfume compositions in which these particularly warm-floral, discretely spicy-oily and very powerful notes are desirable, e.g. modern mossy-balsamic, Oriental-floral, or herbaceous-mossy-aldehydic types.

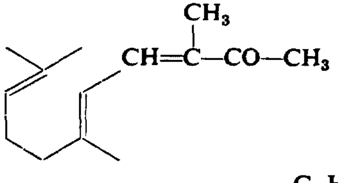
The subject material(s) blend very well with rose bases, balsamic notes, Vetiver and Oakmoss products, etc. and they are very stable in soap. They show less tendency of oxidizing a perfume (or its alcohol solvent) than do the Ionones.

Prod.: by condensation of Citral with Methyl ethyl ketone. The resulting product will normally consist of a mixture of approximately 65% Pseudo-*normal*-methyl ionone and 35% Pseudo-*iso*-methyl ionone (see next monograph), but this ratio can be controlled to a considerable degree through proper choice of conditions.

156-216; 163-67; 163-236;

## 2766: PSEUDO-iso-METHYL IONONE

*2,6,9*-Trimethylundeca-*2,6,8*-trien-*10*-one.
The material exists in *cis*- and *trans*-forms.



$C_{14}H_{22}O = 206.33$

Pale straw-colored or almost colorless oily liquid. Sp.Gr. 0.90. B.P. 268° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, sweet-and-dry-woody, mildly spicy and warm odor of great tenacity. Considerable variations in odor are observed in materials from different suppliers. Traces of Methylionones will strongly influence the odor. See also remarks on this subject in previous monograph (Pseudo methyl-*normal*-ionone).

The title ketone finds some use in perfume compositions where special effects in woody, woody-floral and mossy fragrance types are wanted. In spite of the fact that Pseudo methylionones are very well known, it is surprising to observe how few perfumers actually use pure Pseudo methylionones as tools in creative fragrance work.

Certain commercial perfume specialties are partly based upon Pseudo methyl ionones.

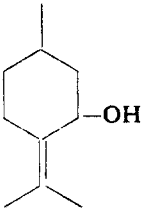
Prod.: by condensation of Citral with Methyl ethyl ketone. The title ketone will – under normal conditions – constitute only about 35% of the total Pseudo methyl ionone mixture. It is possible to change this ratio considerably through variations in the process conditions.

Pseudo methyl-*iso*-methyl ionone is also known.

33-1115; 156-216; 163-67; 163-236; 163-324;

## 2767: PULEGOL

*1*-Methyl-*4*-*iso*-propylidene cyclohexanol-*3*.
*para*-Menthen-*4*-(*8*)-ol-*3*.



$C_{10}H_{18}O = 154.25$

*dextro-trans*-Pulegol: M.P. 76° C. B.P. 212°C.
*laevo-cis*-Pulegol: M.P. 25° C.
Colorless or white crystals, melting to a colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, herbaceous, sweet-minty, rosy odor of moderate to poor tenacity.

Pure Pulegol is not a commercial article and has not been in demand by the creative perfumer. It remains a scarce material in the research laboratory and perhaps in smaller quantities in the essential oil laboratories, for experiments with reconstituted essential oils.

The material is included in this work to elucidate some of the problems, often encountered in perfumery literature when the names Pulegol, Pulegyl acetate, *iso*-Pulegol, *iso*-Pulegyl acetate etc. are mentioned.

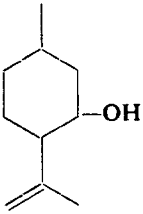
The title material is not yet of interest to the perfumer or the flavorist, and it has not been identified in any significant amount in the natural products used in perfumes or flavors. It may be a natural intermediate in the biogenesis of Menthol via Pulegone.

Prod.: by reduction of *dextro*-Pulegone with Lithium Aluminum hydride.

85-103;

## 2768: iso-PULEGOL

*para*-Menth-*8*-en-*3*-ol.
*1*-Methyl-*4*-*iso*-propenyl cyclohexan-*3*-ol.
A number of stereo-isomers are known, resembling the group of stereo-isomer Menthols:
*laevo-iso*-Pulegol.
*dextro-iso*-Pulegol.
*dextro-neo*-Pulegol.
*dextro-neo-iso*-Pulegol.



$C_{10}H_{18}O = 154.25$

Colorless liquid. Sp.Gr. 0.92 (average data for commercial *iso*-Pulegol). B.P. 201° C.

Very slightly soluble in water, soluble in alcohol and oils.

Minty-herbaceous, bitter-sweet odor of moderate tenacity.

Bitter, rather sharp taste at concentrations higher than 50 ppm. Herbaceous-bitter or bitter-sweet, minty taste near 10 ppm.

This material is used in perfume compositions as a "lift" to Rose notes, Geranium notes, Reseda and Oriental types, various floral fragrances, including Tuberose, etc.

It is also used in flavor compositions in concentrations equal to 5 to 30 ppm in the finished product. The application is mainly in the minty types and in a few Berry flavor types.

G.R.A.S. F.E.M.A. No.2962.

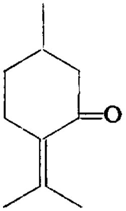
Prod.: from Citronellal via Citronellal-enol. The conventional method involves treatment of Citronellal with Acetic anhydride. *iso*-Pulegyl acetate is the end result. *iso*-Pulegol is an intermediate in the process of making synthetic Menthol (from Citronellal-source).

Newer methods are based upon treatment of Citronellal with boric acid, followed by cyclization by UV-light.

67-520; 88-105; 163-40; 163-67; 163-211; 156-115;

## 2769: PULEGONE

*para*-Menth-*4*(*8*)-en-*3*-one.
*1*-Methyl-*4*-*iso*-propylidene-*3*-cyclohexanone.
The *dextro*-isomer is the most common form.
*laevo*-Pulegone is rarely offered commercially.



$C_{10}H_{16}O = 152.24$

Colorless oily liquid. Sp.Gr. 0.94.
B.P. 224° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and relatively diffusive, herbaceous-minty, resinous odor. The material isolated from Pennyroyal oil (practically all commercial Pulegone is manufactured by that isolation method) may carry more or less of a weedy-bitter note which is not typical of the ketone itself. A highly purified Pulegone is rather sweet, although it does have a weedy-minty character.

Apart from occasional use in artificial essential oils, the ketone does not find much use in perfumery. The natural parent material, Pennyroyal oil, is frequently used and highly appreciated by certain schools of perfumers for use as a powerful soap perfume ingredient. It performs extremely well in herbaceous Fougère type fragrances, Lavender and Lavender-spice compositions, etc.

The title ketone is occasionally used in flavor compositions, mainly as a modifier in Peppermint flavors – to add "spicy notes" and power. The concentration normally used is equivalent to 5 to 30 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2963.

Prod.:

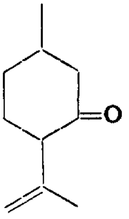
1) by isolation from Pennyroyal oil, usually the Moroccan or the Spanish type.
2) synthetic from *3*-Methyl cyclohexanone. This method will also produce some *iso*-Pulegone.

Pulegone produces Menthol by reduction with nascent Hydrogen.

31-89; 67-526; 89-228; 163-67; 163-236;

# 2770: iso-PULEGONE

*para*-Menth-*8*-en-*3*-one.
*1*-Methyl-*4*-*iso*-propenyl-*3*-cyclohexanone.



$C_{10}H_{16}O = 152.18$

Colorless liquid which turns yellowish when exposed to air and sunlight. It is easily isomerized to Pulegone (see previous monograph). Sp.Gr. 0.93. B.P. 208° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful minty-woody, mildly green odor. Very diffusive and penetrating, not as sweet as Pulegone, not as tenacious.

Refreshing, minty-herbaceous taste in concentrations below 40 ppm, but rather sharp-bitter beyond that level.

The subject ketone may not be a commercial article at all. Literature is still not in agreement with earlier statements that *iso*-Pulegone accompanies Pulegone in Pennyroyal oil, and therefore is rather common. And the subject ketone is rarely found in the pricelists from the suppliers of perfume and flavor chemicals.

The ketone is mentioned in this work mainly to emphasize this doubt about the existence (as a commercial product) and importance (as an individual aroma material) of *iso*-Pulegone.

It may be used in the artificial reconstruction of Geranium and other oils. It is specifically listed in the American G.R.A.S. list of food flavor chemicals, and its use in various types of fruit, berry and mint type flavor is commonly discussed. The level of concentration in finished products would normally be about 5 to 15 ppm.

G.R.A.S. F.E.M.A. No.2964.

Prod.:

1) possibly as part of "total Pulegone" by isolation from Pennyroyal oil.
2) synthetic from *3*-Methyl cyclohexanone (both isomers).

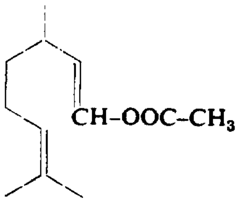
67-526; 89-241; 163-211; 65-404;

# 2771: iso-PULEGYL ACETATE

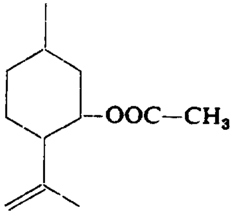
*1*-Methyl-*4*-*iso*-propenyl cyclohexan-*3*-yl acetate.

"Acetylated Citronellal".

The product usually sold under the name "*iso*-Pulegyl acetate" is mostly Citronellal-enol acetate, and there has been much discussion on the subject of nomenclature for the title material.



Citronellal-enol-acetate



*iso*-Pulegyl acetate.

$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. Sp.Gr. 0.93. B.P. 232° C.

Practically insoluble in water, soluble in alcohol and oils.

Fresh, green-minty, leafy, sweet-fruity (unripe fruit) odor of moderate tenacity. The odor of the enol-acetate is sharper, more green, while the *iso*-Pulegyl acetate has a condiment-spicy character, sometimes almost Dill-pickle-like. The title material is rather unstable and undergoes change in chemical composition and in odor, particularly if exposed to sunlight.

The title material is used in perfume compositions as a freshener in Rose, Geranium, Oriental, Lavender, Fougère, etc., particularly in soap where its powerful "lift" is appreciated.

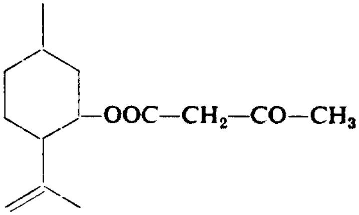
The ester is also used in flavor compositions, mainly Berry- and fruit types, at the rate of 5 to 25 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2965.

Prod.: by cyclization of the Acetate (-enol-acetate) obtained from Citronellal and Acetic anhydride. The enol-acetate is an intermediate in the process of making the title material.

35-503; 156-115; 163-40; 163-211; 163-236; See also monograph: Citronellal enol acetate.

## 2772: iso-PULEGYL ACETOACETATE



$C_{14}H_{22}O_3 = 238.33$

Colorless, slightly oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

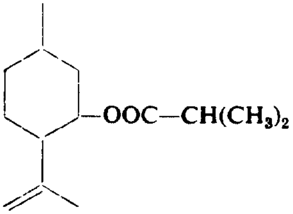
Fruity-green, winey-minty, refreshingly herbaceous odor of moderate tenacity.

The title ester is very rarely offered commercially under its proper chemical name, although it is in no way a chemical secret. It is probably appreciated more by certain perfume houses than by others, and only a few will manufacture this material, all for own use in bases and specialties.

It adds a pleasant "natural"-herbaceous, fresh-winey, mellowness to light floral fragrances, green-winey topnote compositions, delicate Rose or Muguet types, etc. and it gives interesting effects with Citrus oil combinations.

Prod.: e.g. from *iso*-Pulegyl chloride and Malonic ester, followed by careful saponification of the Ethylester.

## 2773: iso-PULEGYL-iso-BUTYRATE



$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid.

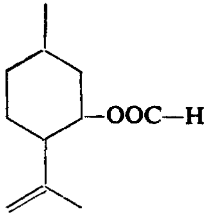
Insoluble in water, soluble in alcohol and oils.

Spicy-sweet, green-leafy and fruity odor of moderate to good tenacity.

This rare ester has been suggested for use in perfume compositions. It is not only a rare ester, but there has been very little demand for it, and the perfumers in general show absolutely no interest in experimenting with the subject ester. It does not offer any very unusual or original fragrance notes other than those which can be obtained by use of conventional chemicals.

Prod.: from Citronellal and *iso*-Butyric anhydride. It has also been prepared directly from *iso*-Pulegol with *iso*-Butyric acid under azeotropic conditions, but the products from the two processes have distinctly different odor.

## 2774: iso-PULEGYL FORMATE



$C_{11}H_{18}O_2 = 170.25$

Colorless mobile liquid. Sp.Gr. 0.96.
B.P. 226° C.

Almost insoluble in water, soluble in alcohol and oils.

Fresh-green, minty, slightly earthy odor of moderate tenacity.

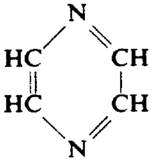
This ester has been suggested for use in perfume compositions as part of Reseda-bases, Rose variations, etc. where the fresh-minty leafy notes are compatible.

The material is very rarely offered commercially, and not often found on the perfumer's shelf. It is reasonable to say that this ester is dispensable and probably almost obsolete in perfumery.

7-225; 163-40; 163-211;

## 2775: PYRAZINE

*para*-Diazine.
Piazine.



$C_4H_4N_2 = 80.09$

Colorless or yellowish crystals or waxy crystalline mass. M.P. 56° C. Sp.Gr. 1.03. B.P. 118° C. Sublimes at room temperature.

Soluble in water, alcohol and most oils.

Pungent, sweet odor, in dilution floral with remote resemblance to Heliotrope. Very diffusive, poor tenacity.

This material has been suggested for use as a trace ingredient in perfume bases, particularly in floral topnotes for heavy, tropical-type florals, etc.

There has been some reluctance on the part of the perfumers, to use this material, and it is quite understandable. Yet, on the other side, many related materials are used in perfumes, e.g. Pyridine, Piperidine, alkyl-Pyridines and Nicotinic esters, etc.

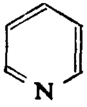
It is again a question of concentration and the proper use of effective, but safely low proportions of such materials, until solid proof is brought about, that the material is safe for cosmetic use below a certain level. The establishment of "safe level" is, naturally, a time-consuming, costly, very subjective and difficult task.

Having been identified as a component of the volatile portion of roasted Coffee, the title material may eventually be used as part of flavor compositions for the reconstitution of Coffee flavor in Coffee extracts. The material is not listed as G.R.A.S. in the USA.

Prod.: (many methods) e.g. by vapor-phase, catalytic dehydration and dehydrogenation of Ethanolamine (or Diethylene triamine).

26-668; 69-1320; 100-875; B-XXIII-91; 157-442;

## 2776: PYRIDINE



$C_5H_5N = 79.10$

Colorless mobile liquid. Sp.Gr. 0.98.
B.P. 115° C. (it boils with water at 92° C.).

Miscible with water, alcohol, Propylene glycol, Glycerin and most oils.

Pungent, penetrating and diffusive odor, generally described as nauseating, but in extreme dilution warm, "burnt", smokey, of very poor tenacity.

It should be kept in mind, that commercial grade Pyridine contains at least 1% *alpha*-Methylpyridine (Picoline) and perhaps other by-products, all higher boiling than Pyridine, and therefore particularly conspicuous as terminal odors on a perfume blotter test. The odor of these derivatives will also heavily influence the overall odor picture of Pyridine.

On the other hand, the most important use of Pyridine is that of being part of the Coffee flavor for reconstitution of the flavor in Coffee extract. Pyridine is a component of the volatile aroma of roasted Coffee, and so are many derivatives and related chemicals. One might therefore assume that a highly purified Pyridine is not absolutely necessary for such purpose.

The taste of Pyridine at concentrations near 1 ppm is rather sharp, burnt, but when accompanied by the volatile aroma of Coffee or Chocolate, it is not unpleasant or out of place.

Pyridine is used in Chocolate flavors and the concentration is usually about 0.02 to 1 ppm in the finished product.

The author is not aware of any significant use of Pyridine in perfumes.

G.R.A.S. F.E.M.A. No.2966.

Pyridine vapors are considered approximately 40 or 50 times less toxic than Benzene vapors. Which is, to a toxicologist, still not very comforting.

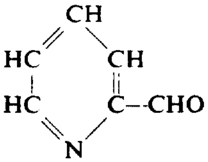
Prod.: Mainly by extraction from coal tar with Sulfuric acid. Pyridine is present in coal tar at the rate of about 0.2%.

Pyridine is also present in tar oil from bone or other animal matter.

69-488; 69-514; 100-876; 157-442;
B-XX-181;

## 2777: PYRIDYL-2-METHANAL

Pyridine-*2*-aldehyde.



$C_6H_5NO = 167.11$

Colorless mobile liquid. B.P. 181° C.

Slightly soluble in water, soluble in alcohol and oils.

Hygroscopic and easily oxidizable to the carboxylic acid when exposed to air.

Pungent Bitter-almond-like odor of poor tenacity. Not quite as stinging as Benzaldehyde, but slightly more bitter, unnatural. In extreme dilution quite pleasant, sweet, Bitter-almond and nut-like.

The title aldehyde has been suggested as a fragrance material for use as a modifier for Benzaldehyde in technical perfumes, masking odors, etc. for industrial purposes.

The Pyridyl-*2*-aldehyde is, however, just as unstable to air (oxygen) as is Benzaldehyde, and it is furthermore hygroscopic. It is not a good substitute for Benzaldehyde, and it does not have economic advantage over that material.

In view of the mentioned considerations, one must assume that the material is obsolete in perfumes and flavors.

It is interesting to note that the material is at the same time an Amine and an Aldehyde. Its Schiff's base has not been mentioned in perfumery literature.

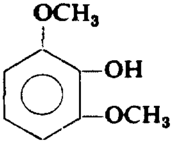
Prod.:

1) from the Schiff's base of *para*-Nitroso dimethylaniline and *2*-Methylpyridinium iodide.
2) by ozonolysis of *2*-Stilbazole.

69-553;

## 2778: PYROGALLOL DIMETHYLETHER

*1,3*-Dimethoxy-*2*-hydroxybenzene.
*2,6*-Dimethoxyphenol.
Pyrogallol-*1,3*-dimethylether (the *1,2*-dimethylether is uncommon).



$C_8H_{10}O_3 = 154.17$

White or colorless crystals. M.P. 55° C.
B.P. 262° C.

2% soluble in water, soluble in alcohol, oils and aqueous alkali.

Woody-medicinal, rather dry odor of considerable tenacity.

The odor is not exactly desirable, but it may find use as part of complex notes such as Oakmoss or certain woods, or the material may be a trace ingredient in Fougères, etc.

Since Pyrogallol itself is toxic and hazardous to human skin, there has been a general reluctance in the use of the ethers. The Trimethylether is used for its dermatological effect, and it is considered much less hazardous than Pyrogallol.

The material is also included in this work in order to further elucidate the name and identity of the chemical, since confusion with Catechol dimethylether (in Europe called Pyrocatechin dimethylether) is possible.

The fact that the title material is a natural component of natural and processed-natural materials (essential oils and Beech tar creosote) is no guaranty that it is harmless.

It is also interesting to note that Pyrogallol-*1*-methylether is a starting material in the synthesis of Myristicin, one of the toxic elements in Nutmeg oil.

Prod.:

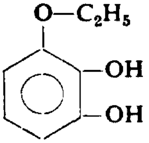
1) from Pyrogallol in aqueous alkali with Methyl iodide.
2) from Pyrogallol trimethylether by demethylation with alkali in water or alcohol.

   Pyrogallol trimethyl ether is prepared the conventional way from Pyrogallol with Dimethylsulfate in cold, diluted Sodium hydroxide solution.

67-480; 90-387; 100-880;

## 2779: PYROGALLOL MONOETHYLETHER

Pyrogallol-*1*-ethylether.
*1*-Ethoxy-*2,3*-dihydroxybenzene.



$C_8H_{10}O_3 = 154.17$

White crystals or fused mass.

Very slightly soluble in water, soluble in alcohol, oils and aqueous alkali.

Dry-woody, very tar-like odor, but not unpleasant in dilution. Also smokey, resembling odor of wood-fire, with no petroleum-tar type odor. Very good tenacity.

The title material is occasionally used as part of "Beech wood" or "Beech tar" (creosote) notes in "leather" type fragrances. It will blend well with Oakmoss and Labdanum for such purposes, but it tends to discolor when exposed to daylight, and only very low concentrations in the final fragrance are fairly safe against this drawback.

See also monograph: Creosote. See comments on dermatological effect under Pyrogallol dimethylether, preceding this monograph.

Prod.: by controlled Ethylation of Pyrogallol in weak aqueous alkaline solution with Diethyl sulfate.

3-207; 4-234; 163-115;

## 2780: PYROLIGNEOUS ACID

"Liquid Smoke" (old, commercial name).
Wood vinegar.
Pyroligneous vinegar.

The title material is not a well defined, single chemical. Its chief component is water, and its chief active ingredients by volume are Formic acid, Acetic acid and Propionic acid. The acid content is usually near 10%.

It is miscible with water and alcohol, but not with oils. It is also miscible with Propylene glycol. The material and its solutions will often separate oil droplets of a tar-like substance upon standing. The tar-like phase is insoluble in water and diluted alcohol.

Pyroligneous acid is manufactured by destructive distillation of wood, preferably Birch wood, of which Sweden is a major producer.

The crude or filtrated Pyroligneous acid is used in the flavoring of meats, fish and other preserves, and to a lesser extent in flavor compositions for imitation Caramel, Butterscotch, Rum, Vanilla, etc. and in tobacco flavorings.

The concentration of the title material in finished consumer products may be between 10 and 300 ppm, highest in "smoked" meat and fish products.

For special purposes, and to facilitate blending into ordinary flavor compositions, a PYROLIGNEOUS ACID EXTRACT is also manufactured. It is free from water, acid and tar, produced from crude Pyroligneous acid by alkali washing, re-acidification and selective solvent extraction.

Pyroligneous acid extract is used as a "smoke" flavor in such compositions, and finds end-use in meat and fish products only. The concentration of this material in functional products is normally about 20 to 300 ppm, highest in certain fish products.

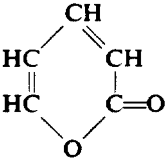
Pyroligneous acid: G.R.A.S. F.E.M.A. No.2967.

Pyroligneous acid extract: G.R.A.S.

100-881; 104-565;

## 2781: alpha-PYRONE

Coumalin.
*2*-Pyrone.
*1*,*2*-Pyrone.



$C_5H_4O_2 = 96.09$

Colorless or pale straw-colored oily liquid. Solidifies in the cold, melts again at +5° C. B.P. 209° C.

Polymerizes easily upon standing, particularly under alkaline conditions.

Very slightly soluble in water, soluble in alcohol and oils.

Pleasant hay-like, herbaceous-warm odor of moderate to poor tenacity. The hay-like notes are more coumarinic than those of *2*-Methyl pyrone.

This ketone has been suggested for use in perfume compositions as a modifier for Coumarin and coumarinic materials (Heptalactone, etc.). It would undoubtedly be a valuable candidate for further experiments in Fougères, Chypres, Lavender and Citrus compositions, if it were not for its sensitivity to alkali, iron and daylight. The polymerized Pyrone is practically odorless and of dark color.

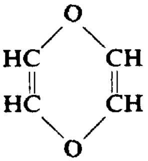
It is interesting to note that Pyrone is an empirical isomer of Furfural.

Prod.: from Diethyl oxalate plus Ethyl crotonate via *2*-Pyrone-*6*-carboxylic acid. Decarboxylation of that acid yields the title ketone.

1-557; 3-190; 69-819; 140-174;

## 2782: gamma-PYRONE

*1,4*-Pyrone.



$C_5H_4O_2 = 96.09$

Colorless crystals. M.P. 32° C. B.P. 216° C.

Slightly soluble in water, soluble in alcohol and oils.

Polymerizes under exposure to air (oxygen) and alkali. Turns darker brown, and its odor fades.

Warm, slightly pungent, hay-like herbaceous odor of moderate to poor tenacity. Sharper than the odor of *alpha*-Pyrone, and not quite as hay-like as that isomer.

The title material as such finds very little use in perfumes or flavors, but it is a very important intermediate (in Nature, particularly) in the synthesis of many interesting flavor materials.

Hydroxy-*gamma*-pyrones and their derivatives include Maltol, Ethyl Maltol, Kojic acid, Dehydroacetic acid, etc. all naturally occurring in food products, and also used in flavor compositions.

If it were not for the rather poor stability of the title material, it could undoubtedly find use in perfumes and flavors as a modifier for Coumarin in Fougères and Lavender perfumes, and in Nut, Rum, Bread, Caramel and many other flavor types.

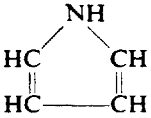
Prod.:

1) from Diethylacetone dioxalate by cyclization to Chelidonic acid (*gamma*-Pyrone-*2,6*-dicarboxylic acid). The acid yields the title material by decarboxylation.
2) by heating of *1*-Methoxypent-*1*-en-*3*-yn-*5*-al diethylacetal with Methanol and water, using Mercuric sulfate or Sulfuric acid catalyst.

1-560; 1-808; 69-827; 69-833;

## 2783: PYRROLE

Azole.
Imidole.
Divinylenimine.



$C_4H_5N = 67.09$

Colorless liquid, but turns brown under exposure to air (oxygen) and is easily oxidized. Sp.Gr. 0.97. B.P. 131° C. (decomposes). Material should be distilled under vacuum only.

8% soluble in water, miscible with alcohol and oils.

Sweet and warm-ethereal, slightly burnt-nauseating odor, resembling the odor of Propyl formate. The odor of Pyrrole is often described in chemical literature as resembling that of Chloroform, but the author believes that perfumers generally will have difficulty in finding much similarity between the two.

The title material has been suggested for use in masking odors for industrial purposes, and it may serve a purpose of masking if the undesirable odor is of approximately the same volatility as Pyrrole. However, the poor stability of Pyrrole under the normally rough conditions for industrial masking make it rather difficult to justify the use of this material at all. The title material has also been suggested for use as a trace ingredient in artificial Petitgrain oils.

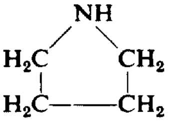
Prod.:

1) by fractionated distillation of bone oil.
2) by thermal decomposition of Ammonium mucate with Glycerin or mineral oil.

7-333; 7-335; 100-882; 159-431; 159-434; B-XX-159; 90-809; 31-278;

## 2784: PYRROLIDINE

Tetrahydro pyrrole.



$C_4H_9N = 71.12$

Almost colorless liquid. Sp.Gr. 0.85.
B.P. 89° C.

Miscible with water, alcohol and most oils.

Penetrating Amine-type odor, reminiscent of Ammonia and Piperidine, nauseating and diffusive, of very poor tenacity.

The liquid fumes in air and has strongly alkaline reaction.

Although the title amine has been identified in Tobacco leaves and Carrot leaves, it has failed to find use in perfume and flavor compositions. Its volatility and repulsive odor make it difficult to use, even with strong fixation. Traces of the title material may be used in artificial flower absolutes and certain artificial essential oils, exotic flower bases, etc. It performs well with Methyl phenylethylether for such purpose.

Prod.: by hydrogenation of Pyrrole with Hydrogen iodide plus Phosphorous, or with Hydrogen in presence of Adams catalyst (Platinic oxide).

1-785; 26-670; 69-62; 100-882; B-XX-4;

## 2785: PYRUVIC ACID

*alpha*-Ketopropionic acid.
*2*-Oxopropanoic acid.
Pyroracemic acid.
Acetylformic acid.

$CH_3—CO—COOH$

$C_3H_4O_3 = 88.07$

Colorless viscous liquid, solidifying in the cold. M.P. 13° C. Polymerizes easily and acquires a brownish color and caramellic odor. Sp.Gr. 1.26. B.P. 165° C under decomposition.

Miscible with water, alcohol and oils.

Sour-acetic odor. Pleasant sour taste, accompanied by a mildly burnt note which gives the impression of caramellic sweetness.

The title acid is not used in perfumes.

It finds extensive use in flavor compositions, mostly in the form of esters. The acid itself is used in imitation Coffee and Rum flavors at concentrations equal to 1 to 30 ppm in the finished product. The concentration in chewing gum may be as high as 110 ppm.

The Amino-acid Alanin is produced in the human liver from Pyruvic acid. By loss of Carbon dioxide, the title acid forms Acetaldehyde. This is one of many processes taking place in the making of wine and Brandy.

G.R.A.S. F.E.M.A. No.2970.

Prod.:

1) from Tartaric acid by heating with hydrophilic agents, such as Potassium hydrosulfate.
2) from Acetyl chloride and Potassium cyanide. The resulting Pyruvic nitrile is acid hydrolyzed to the title acid. Pyruvic acid must be rectified in vacuum.

1-269; 26-670; 100-882; 140-148; B-III-608;

## 2786: PYRUVIC ALDEHYDE

*1,2*-Ketopropionic aldehyde.
*2*-Oxopropanal.
Acetyl formaldehyde.
Methyl glyoxal.
*alpha*-Ketopropionic aldehyde.
Pyruvaldehyde.

$CH_3—CO—CHO$

$C_3H_4O_2 = 72.07$

Hygroscopic, yellow, mobile liquid.
Sp.Gr. 1.05. B.P. 72° C.

Easily polymerized if exposed to air. The polymer is a viscous, non-pourable material.

Pungent, stinging odor, very diffusive and of poor tenacity.

Aqueous and alcoholic solutions are colorless, while the solutions in oils (flavor materials, if colorless) are yellowish.

The taste is pungent-caramellic, but also sweet in concentrations below 5 ppm. Higher concentrations give impression of acid sweetness.

The title aldehyde is used in minute traces in imitation Coffee, Maple, Honey, Caramel and Rum flavors. The concentration in finished products is seldom higher than 1 ppm.

Prod.: (many methods) e.g.:

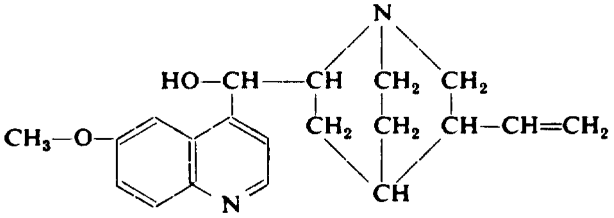
1) by oxidation of Acetone with Selenium dioxide.
2) by heating of Dihydroxyacetone with Phosphorus pentoxide.
3) by warming of *iso*-Nitroso acetone with dilute sulfuric acid.

etc.

G.R.A.S. F.E.M.A. No.2969.

66-718; 100-882;

# 2787: QUININE



$(+3H_2O)$

$C_{20}H_{24}N_2O_2 = 324.43$
(anhydrous)

Dull, needlelike, bulky crystals, colorless or white, but turning brownish upon exposure to air.

M.P. 177° C. (decomposes).

0.05% soluble in water, 0.14% in boiling water, soluble in alcohol and oils, but poorly soluble in most hydrocarbons.

The solution in very diluted Sulfuric acid shows blue fluorescence.

Practically odorless. Intensely, but very "clean", bitter taste. The bitterness is perceptible at concentrations down to 5 or 2 ppm, but this minimum perceptible level is highly subjective. The highest "pleasant level" is near 100 ppm, depending very much upon the acidity accompanying the Quinine bitterness. Without accompanying acid, the pleasant level is much lower.

Quinine (alkaloid) is rarely used as such in flavors, but several of its salts are used in flavors and beverages as an additive. The word "Quinine" is commonly used to cover the use of one or another salt of the alkaloid.

More than fifty salts of Quinine are commercially available. Three are listed in the American G.R.A.S. list:

Quinine monohydrochloride ("Quinine chloride").

Quinine monosulfate ("Quinine sulfate") – – and

Quinine bisulfate.

The American authorities allow a maximum of 83 ppm (calculated as Quinine alkaloid, base) in carbonated beverages. There are countries, where the use of Quinine in carbonated beverages is prohibited. Bitter effect in "Quinine water" must then be achieved by other chemicals (Naringin, etc.). See comments under monograph Quinine bisulfate about safe level.

Prod.: by extraction from the bark of Cinchona officinalis (commonly known as "Ledgeriana-bark" or "Cinchona bark") in which the alkaloid is present at the rate of up to 8%.

1-877; 69-1893; 100-888; 124-323; 159-267;

# 2788: QUININE BISULFATE

Structure: see monograph: Quinine.

$C_{20}H_{24}N_2O_2—H_2SO_4+7H_2O = 548.62$

Crystals or crystalline powder. White when fresh, but may acquire a brownish tint upon exposure to air.

10% soluble in water, 4% in alcohol, 6% in Glycerin. The saturated aqueous solution has acid reaction ($p_H = 3.5$).

Odorless, but has intensely bitter taste.

This salt is used as a bitter additive to beverages, mostly carbonated beverages, and usually accompanied by a food acid. The combination of sour and bitter taste impression is far more pleasant to the human organoleptic receptacles than the bitter stimulus alone.

The concentration normally found in beverages is about 100 ppm, which is near the maximum permissible (83 ppm of Quinine base) in the U.S.A. Since the hazardous dose of Quinine is over 1.5 grams (per dose), it would be necessary to consume 20 Litres (about 5 U.S. gallons) of such beverage to achieve a total of a hazardous single dose.

Not only is it unlikely that anyone can consume 20 Litres within, say, one hour, but it is most inconceivable that such quantity could be consumed within a 24-hour period. And the maximum daily dose of Quinine is several times higher than 1.5 grams (hazard-level).

G.R.A.S. F.E.M.A. No.2975.

100-889; The reader is referred to conventional pharmaceutical literature for detailed description of the Quinine alkaloid and its salts.

## 2789: QUININE HYDROCHLORIDE

Quinine chloride.
Quinine monohydrochloride.
Structure: see monograph: Quinine.

$C_{20}H_{24}N_2O_2, HCl+2H_2O = 396.93$

Shiny, silky, needle-like colorless or white crystals.

6% soluble in water, 50% soluble in alcohol, 12% soluble in Glycerin. Aqueous solutions are almost neutral.

Odorless. Intensely bitter taste.

This Quinine salt is used in various Bitters, in Citrus and fruit flavors for candy, beverages, etc. Its excellent solubility in water and alcohol makes it very suitable for incorporation in flavor compositions.

The normal concentration of this salt in finished goods is about 110 ppm, which is very near the maximum permissible (83 ppm calculated as Quinine alkaloid) in the U.S.A.

For further comments on safe concentration and hazard levels, see monographs on Quinine and Quinine bisulfate, preceding this monograph.

G.R.A.S. F.E.M.A. No.2976.

100-892;

## 2790: QUININE SULFATE

Structure: see monograph: Quinine.

$(C_{20}H_{24}N_2O_2)_2—H_2SO_4+7H_2O = 873.05$

White, dull, needle-like crystals.

0.12% soluble in water, 0.9% soluble in alcohol.

The aqueous solutions are almost neutral.

Odorless. Intensely bitter taste.

Quinine sulfate is used for the same purposes as described under Quinine hydrochloride. The latter is often preferred for its better solubility, but the normal use level does not bring the salt to a concentration where solubility becomes a real problem.

The title material is used as a bitter matter in carbonated beverages, candy and certain other foods. The concentration in beverages is normally about 100 ppm, which is equivalent to 0.03 grams of Quinine sulfate in a medium-size bottle (300 ml.). One Litre of such beverage would contain enough Quinine sulfate to make a perceptible physiological effect upon an adult person.

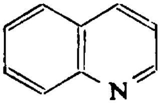
The concentration is, however, well below the hazardous level, which is described more detailed under monograph: Quinine. There has been a tendency of using bitter matter other than Quinine in bitter beverages, partly because of the fluctuations in supply of the alkaloid, partly because of the high cost of Quinine as compared to Quassia or Naringin or other bitter additives. It should be kept in mind however, that the above dosage of Quinine will unquestionably have a tonic effect upon the human system, while such effect can not be achieved with Naringin or Quassia.

G.R.A.S. F.E.M.A. No.2977.

100-892;

# 2791: QUINOLINE

*1*-Benzaline.
*2,3*-Benzopyridine.
Chinoleine.
Leucoline.



$C_9H_7N = 129.16$

Colorless, hygroscopic liquid. Darkens upon storage. Sp.Gr. 1.10. B.P. 238° C.

0.6% soluble in water, soluble in hot water, miscible with alcohol and oils.

Heavy, penetrating and nauseating, yet sweet odor of good tenacity. Not as pungent-diffusive as Pyridine, not nearly as anisic as *iso*-Quinoline (see next).

The aqueous solutions are slightly alkaline.

This material is occasionally used in trace amounts in perfume bases, artificial flower absolutes, etc. where its heavy sweetness may introduce certain amounts of the warm-floral notes, difficult to obtain with conventional materials.

The *iso*-Quinoline is generally preferred, particularly since it is also an approved flavor chemical. There is a considerable difference in the odor of the two Quinolines.

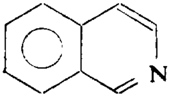
The title material is not permitted for food flavors in the U.S.A.

Prod.: (many methods) e. g. by Skraup's synthesis from Aniline, Glycerol, and Nitrobenzene in the presence of sulfuric acid.

1-815; 69-587; 69-602; 100-893; 159-432; B-XX-339;

# 2792: iso-QUINOLINE

*2*-Benzazine.
*3,4*-Benzopyridine.
*2*-Azanaphthalene.



$C_9H_7N = 129.16$

Colorless hygroscopic, plate-like crystals. M.P. 27° C. The liquid material is almost colorless, slightly viscous. Sp.Gr. 1.09 (liquid). B.P. 243° C.

Slightly soluble in water, miscible with alcohol and oils.

The aqueous solutions are more alkaline than those of Quinoline.

Heavy-sweet, balsamic-herbaceous odor with some resemblance to Benzaldehyde and Anethole.

The taste in concentrations below 5 ppm is sweet, herbaceous-balsamic and warm, very slightly floral, and pleasantly animal-like.

The title material is occasionally used in perfume compositions as a trace ingredient in artificial flower absolutes, certain heavy-floral, balsamic or Oriental-animal bases, musk compositions, etc.

It is also used in flavor compositions, although almost exclusively in imitation Vanilla flavor. The concentration used is equivalent to about 0.2 to 1 ppm in the finished product. The subject material blends well with Castoreum, Creosol, Perubalsam, etc. for such purpose.

G.R.A.S. F.E.M.A. No.2978.

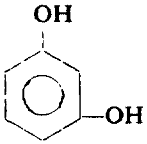
Prod.:

1) by isolation from coal tar. It represents 1% of the total Quinoline fraction.
2) by extraction from Petroleum distillates.

1-815; 69-645; 69-654; 100-581; 159-432;

## 2793: RESORCINOL

Resorcin.
*meta*-Dihydroxybenzene.
*1,3*-Benzene diol.



$C_6H_6O_2 = 110.11$

White plates, needles or prisms. M.P. 111° C. B.P. 276° C.

The crystals may acquire a reddish tint upon exposure to air.

Practically odorless when pure. Tart-sweet taste in proper dilution in water (moderately toxic).

60% soluble in water, 50% soluble in alcohol, soluble in most perfume and flavor materials, also in Glycerin and Propylene glycol.

The title dihydric phenol is briefly mentioned in this work because it has found some use in products where perfumes or flavors are used, and the Resorcinol itself has been classified as "approved for use as a synthetic flavoring or adjuvant) by the American F.D.A.

Several derivatives of Resorcinol are used in perfumery and flavor compositions.

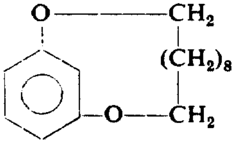
Resorcinol is moderately toxic by ingestion, and aqueous solutions stronger than 10% are considered corrosive to the human skin. However, the use of Resorcinol (as a bactericide, e. g.) requires only very low concentrations of this material.

It is interesting, however, to note that Hydroquinone (*1,4*-Dimethoxy benzene) is also approved by the American authorities, while the third isomer, Catechol (*1,2*-Dimethoxybenzene) is NOT approved for food use.

Prod.: by alkali fusion of *meta*-Benzene disulfonic acid. In the 19th century, Resorcinol was identified after alkali fusion of Galbanum or Asa foetida resins. It is possible that Paeonol or related component of such resins are responsible for the formation of Resorcinol by this alkali fusion.

68-470; 100-901; 162-620; B-VI-796;

## 2794: RESORCINOL DECAMETHYLENE ETHER



$C_{16}H_{24}O_2 = 248.37$

Colorless viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm, musky-woody, mildly nut-like and very tenacious odor.

The title material has been suggested for use in perfumes, but it has, to the author's knowledge, not yet been offered commercially under its proper chemical name.

The ether came out of a research program investigating the cyclic ethers of dihydric phenols. Several materials were suggested for use in perfumes, but the author has included only this material as one example.

It is interesting to compare the structure of these materials with those of the series of ketals, prepared from dihydric phenols (particularly Catechol) and symmetric or asymmetric alifatic ketones, e. g. Di-*iso*-amylketal of Resorcinol. That material has been experimentally produced and appears to have a floral, tenacious odor.

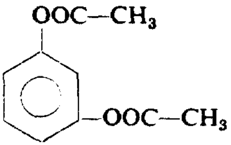
Resorcinol is still considered a relatively expensive starting material – from a perfume chemist's point of view. There is very little chance that these materials will become popular or important in perfumery, unless Resorcinol becomes available at about one-third of the present cost.

Prod.: from Decamethylene dichloride plus Methanol and Sodium methoxide boiled with Resorcinol.

31-153; German patent No. 671840 (1939).

## 2795: RESORCINOL DIACETATE

*1,3*-Diacetyl resorcin.



$C_{10}H_{10}O_4 = 194.19$

Yellowish or pale straw-colored viscous liquid. B.P. 275° C. (decomposes).

Very slightly soluble in water, soluble in alcohol and oils.

Refreshingly woody-mossy odor of good tenacity. Older samples may show acid or acetic notes, not typical of the pure acetate. This apparent instability may be one reason for the lack of interest in the material.

The monoacetate is used or has been used in Dermatology, but Resorcinol itself is considered a potential skin-irritant, to be used only under constant supervision of a physician.

The title material was once suggested for use in perfume compositions, but the author can see no advantage in this Acetate over the more conventional and less hazardous materials. Ketals or ethers of Resorcinol are known and several such derivatives are used as perfume or flavor chemicals.

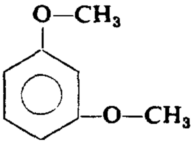
There is reason to believe that the title material is practically obsolete in perfumery.

Prod.: from Resorcinol and Acetic anhydride.

26-672; 68-472; 100-901; B-VI-816;

## 2796: RESORCINOL DIMETHYLETHER

*meta*-Dimethoxybenzene.
"Noisettal".
"Dimethylresorcinol" (see NOTE below).



$C_8H_{10}O_2 = 138.12$

Colorless liquid. Sp.Gr. 1.06. B.P. 215° C.

Slightly soluble in water, soluble in alcohol and oils.

Very powerful, sweet-earthy and intensely nut-like odor, reminiscent of Hazelnuts (or Philberts). The author finds that the odor is better described as resembling that of "old Hazelnuts", just shelled and then crushed.

The flavor is warm-herbaceous, Hazelnut-like and sweet in concentrations below 10 ppm. The flavor tends to become "earthy" at higher concentrations.

This ether – although well known as a chemical – is not very often used in perfume compositions. In fact, it is missing in many perfume laboratories. Its effect with Oakmoss and Vetiver should indeed be tried by every perfumer with imagination and "material audacity". The ether can certainly introduce very pleasant and unusual, inimitable notes to Chypres, Fougères, Clover, Hyacinth, etc. – or simply be a novel additive to a moss-base. It is stable in soap. In fact, it is usually cleaned chemically free from the Mono-ether by washing with a 10% Sodium hydroxide solution. Which is indeed a rough treatment for any perfume material.

The title material is also used in flavor compositions, and it is probably more famous for its aroma-effect than for its fragrance. It is often an important part of Hazelnut imitation flavor, Coconut, Walnut, fruit complexes and it may be used in trace amounts in Vanilla imitation. The concentration of the ether in functional products is normally about 0.5 to 5 ppm.

Prod.:

1) by Methylation of Resorcinol in weak aqueous alkali with Dimethylsulfate.
2) from Methanol and Resorcinol with Potassium hydrosulfate or Sodium naphthalene sulfonate as dehydrating agent.

G.R.A.S. F.E.M.A. No.2385.

68-471; 103-219; 103-306; 140-170; 163-67; SA-private experiments;

Note: There are *four* materials by the name of "Dimethyl resorcinol":

1) *beta*-Orcin = *2,5*-Dimethyl resorcinol.
2) Xyloresorcinol = *4,6*-Dimethyl resorcinol.
3) *3,5*-Dihydroxy-*ortho*-xylene = *4,5*-Dimethyl resorcinol.
4) *2,4*-Dihydroxy-*meta*-xylene = *2,4*-Dimethoxy resorcinol.

None of these are perfume or flavor materials, and they should not be confused with the title ether.

The author takes this opportunity of repeating an old recommendation that the title material be labelled "Resorcinol dimethylether", so that the name "Dimethyl resorcinol" simply is eliminated from the perfumer's mind.

The same could be said about Hydroquinone dimethylether, which is still, stubbornly, labelled "Dimethyl hydroquinone", which is wrong.

The author has more than once seen perfume laboratories with the jar labelled "Dimethyl hydroquinone" under letter "D" on one shelf and the same laboratory with the jar labelled "Hydroquinone dimethylether" under letter "H" on another shelf. Such findings should encourage perfumers who are not chemists to modernize their nomenclature.

One company with the above confusion on laboratory shelves would purchase "Dimethylhydroquinone" from one supplier and "Hydroquinone dimethylether" from another supplier. Thus, a confusion in the perfume laboratory (which should be the example of order and unambiguous nomenclature) may well contaminate the purchasing department of the same company, and from there the confusion will spread to the suppliers, etc. etc.

## 2797: RHODINOL

The name "Rhodinol" has been used to describe single chemicals as well as a group of related chemicals.

In perfumery terms, the name "Rhodinol" most often refers to the professionally composed selection of fractions from vacuum-distilled, or steamdistilled, saponified Geranium oil.

The name "Rhodinol" has at times been used to describe the alcohol which was at one time considered the characteristic and most important alcohol in Geranium oil: *laevo*-Citronellol.

*laevo*-Citronellol is a well-defined chemical and it is described under a separate monograph in this work.

Commercial "Rhodinol" may also be certain grades of Citronellol, or Citronellol obtained by special process.

The commercial product called "Rhodinol C" is usually a purified Citronellol from Citronella oil, while the commercial material "Rhodinol coeur" is a composition of fractions from vacuumdistilled, saponified Geranium oil, normally the Reunion (Bourbon) type.

This type of "Rhodinol" contains *laevo*-Citronellol (in its *beta*-form) as chief component. Other components are Geraniol, *4*-Terpinenol, Linalool, *alpha*-Terpineol, Phenylethylalcohol, etc.

Numerous other alcohols may be present in traces, while the ketone portion is normally excluded or reduced in the composition. The purpose of making "Rhodinol coeur" is to have an extremely rosy-floral, sweet and clean material as a base for many types of floral fragrance, particularly for Muguet.

In fact, the performance in a luxury Muguet perfume may just tell you the difference in quality of the Rhodinol employed.

The flavor chemist may be even more discriminate, since "Rhodinol" is used as a sweet undertone in Strawberry, Raspberry, Currant, Honey, Grape and in fruit complexes, spice blends, Ginger Ale flavor, Chocolate imitation, etc. The concentration is normally about 1 to 10 ppm in the finished product, except in chewing gum, where it may reach 30 ppm.

Rhodinol is an expensive perfume material (about twice the cost of Geranium oil) but it is unsurpassed in floral beauty. It can not be replaced by any grade of Citronellol (synthetic or Citronella-isolate) in a composition.

The single chemical "Rhodinol" (presumably a mixture of *dl-beta*-Citronellol and *l-beta*-Citronellol) would be an extremely expensive material, and so is the synthetic *laevo*-Citronellol (about 5 times the cost of Geranium oil). The perfumers seem to be generally in agreement that the composition of fractions from vacuum- or steam-distilled, saponified Geranium oil is the preferable perfume material and the best base for a Rose or Muguet fragrance.

G.R.A.S. F.E.M.A. No.2980.

31-17; 163-67; 163-236; 104-273; 159-121; 106-314;

## 2798: RHODINYL ACETATE

Acetylated Rhodinol, see monograph: Rhodinol.

Sp.Gr. approximately 0.90.
B.P. approximately 237° C.

Colorless oily liquid. Practically insoluble in water, soluble in alcohol and oils.

Sweet, light and refreshing Rose-Muguet type of odor with variable amounts of delicately green or leafy notes.

Sweet berry-like, fruity taste in concentrations below 20 ppm.

This ester, which represents the mixed acetates of the alcohols available in the commercial product known as Rhodinol (from Geranium oil), is used in perfume compositions, mostly in luxury perfumes. It lends very attractive top- and middle-notes to Muguet, Carnation, Gardenia, Freesia, Rose, etc. and it blends well with Citrus oils, Ionones, fruity and green odors, etc. It is often used in better lipstick perfumes.

The ester is used in flavor compositions in discrete amounts for the sweet berry-types, Strawberry, Raspberry, and in Honey, Rose, Apricot, Coconut imitation. Its use in the old-fashioned "Sen-Sen" type or "Cachou" type fragrance is well known and occasionally transferred to new versions of floral dentifrice flavors. It is sweeter than Geranium oil, but tends to perform very "perfumey" at levels higher than 10 or 20 ppm, particularly in combination with Ionones and Patchouli ("Sen-Sen"-types, etc.).

Normal concentration is from 1 to 20 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2981.

Prod.: by Acetylation of Rhodinol from Geranium oil.

33-504; 106-315; 163-68; 163-236; 103-99;

## 2799: RHODINYL BENZOATE

See monograph: Rhodinol, for composition.

Colorless or very pale straw-colored, slightly viscous liquid. B.P. approximately 338° C. Sp.Gr. approximately 0.98.

Practically insoluble in water, soluble in alcohol and oils.

Mild, but very tenacious, deep-sweet, rosy-balsamic odor.

This ester could serve as a fixative in many perfume types other than Rose, but it is generally far too expensive for such purpose. To achieve a perceptible and truly physical fixation, one would have to use at least 5%, often 10% of the ester, even if considerable amounts of other fixatives were employed in the same fragrance.

With a material cost of about three times the price of Geranium oil, one would have to limit the use of this ester to high-cost perfumes only. And its effect is not so much more attractive than that of Geranylbenzoate, now available in a very fine quality.

Briefly, the title ester is a material of the past, and today's perfumer would undoubtedly know how to make use of Geranyl benzoate or other materials and achieve a fully satisfactory result without the use of Rhodinyl benzoate.

Prod.: by azeotropic esterification of Rhodinol (from Geranium oil) with Benzoic acid.

A product made by alcohol interchange esterification method will have an entirely different odor.

103-132; 163-68; 163-236;

## 2800: RHODINYL-n-BUTYRATE

See monograph: Rhodinol, for composition.

Colorless oily liquid. Sp.Gr. approximately 0.89. B.P. approximately 266° C.

Practically insoluble in water, soluble in alcohol and oils.

Intensely sweet, mellow-fruity, deep rosy odor of moderate to good tenacity. An acid-free ester may have an odor very closely resembling the petals of certain varieties of Rose (petal-odor).

Pleasant, sweet-fruity, mellow-Apple-like taste in concentrations below 10 ppm.

This ester is, next to the Acetate, probably the most popular ester of Rhodinol. Its rich, sweetening effect in light floral fragrances, such as Muguet, Freesia, Peony, etc. is very highly appreciated, but it takes solid experience and a good quality material to achieve such effects. Needless to say that if the ester contains free acid, its odor picture is completely ruined, and many perfumers may have avoided the use of this material because the bottle on the shelf was not used often enough, or not renewed or checked often enough.

In Cassie, Hyacinth, variations of Carnation and in the so-called "Oriental Rose" (often just a warmer, deeper, fruitier type), the title ester finds frequent use.

It is also used in flavor compositions for imitation Apple, Pear, Melon, Plum, Raspberry, Strawberry and in many fruit complexes.

Traces may be used for bouquetting of a dentifrice flavor.

The normal concentration is about 1 to 10 ppm in the finished product.

The author has the impression that the *n*-Butyrate is generally preferred by the perfumers, while the flavorists seem to prefer the *iso*-Butyrate. The two materials are separately approved as G.R.A.S. by F.E.M.A. in the U.S.A.

Prod.: from Rhodinol (ex Geranium oil) and *n*-Butyric anhydride.

33-734; 103-117; 163-68; 163-236;
See also Rhodinyl-*iso*-butyrate (next monograph).

## 2801: RHODINYL-iso-BUTYRATE

For composition, see monograph: Rhodinol.

Colorless oily liquid. B.P. approximately 260° C. Sp.Gr. approximately 0.89.

Delicately fruity, fresh-floral and sweet, tenacious odor. Overall more fresh and delicate than the *n*-Butyrate, but not as natural rosy or "petal-like".

Fruity-floral, intensely sweet taste. Fresher, less deep-heavy than the *n*-Butyrate at same concentration. More towards Pineapple, less Plum-like.

This ester finds some use in perfume compositions, but not nearly as much as the *n*-Butyrate. It is used largely in the same type of fragrance but it does not introduce the same deep-rosy tonality. Only in Muguet it may perform as good or even better.

The ester finds a good deal of use in imitation Apple, Pineapple, Pear, Honey, Raspberry, and in various Rose and other "floral" flavor types. The concentration is normally about 1 to 5 ppm, rarely up to 10 ppm in the finished product.

Prod.: from Rhodinol and *iso*-Butyric anhydride.

G.R.A.S. F.E.M.A. No.2983.

163-68;

## 2802: RHODINYL CINNAMATE

See also: Citronellyl cinnamate.
For composition, see monograph: Rhodinol.

Pale straw-colored, slightly viscous liquid. B.P. approximately 375° C.
Sp.Gr. approximately 0.98.

Insoluble in water, soluble in alcohol and oils.

The title ester is probably not commercially available in a quality which could justly be labelled "Rhodinyl cinnamate".

The commercial product under the title name has a very delicate, refined balsamic, but also very weak, rosy odor of excellent tenacity. The odor has sometimes been described as resembling that of the white rose varieties.

It is hardly conceivable that a material, truly corresponding to the above name, could be commercially interesting. It would be very expensive, and the materials so far marketed under the title name have not caused any enthousiasm among the perfumers.

A fairly pure Citronellyl cinnamate is commercially available.

The author would classify the title material as practically obsolete.

Prod.: A production via alcohol interchange esterification would not lead to a satisfactory ester, but such material has been commercially available a few years ago.

2-1122; 34-484; 103-148; 163-236;

## 2803: RHODINYL FORMATE

For composition: see monograph Rhodinol.

Colorless, mobile liquid. Sp.Gr. approximately 0.91. B.P. approximately 220° C.

Very slightly soluble in water, soluble in alcohol and oils.

Fresh, leafy-green, delicately rosy, yet powerful odor of moderate tenacity.

Pleasant Apricot-and-berry type flavor in concentrations below 10 ppm.

This ester, when properly prepared, acid-free and clean (dry), is an exquisite perfume material. As a topnote material it ranks among the finest and most versatile chemicals. Its refreshing effect can be combined with delicately floral Muguet, with intensely sweet fruity Gardenia, with refreshingly green and earthy Galbanum or Oakmoss.

Larger amounts are used in rose variations, Eglantine or Hip-rose (hedge rose) types, in

Bruyère fantasy, in Carnation or Peony, etc. If Rhodinol puts a delightful "heart" into a fragrance, the formate will supply the "life" and "pulse" of this heart. One material needs the other in order to perform truly attractive.

The ester is used in trace amounts in imitation Raspberry, Apple, Cherry, Plum, Pineapple, Pear, Apricot, Peach, and in Bitter Almond (often along with traces of Bulgarian Rose oil), etc.

The concentration is normally about 1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2984.

Prod.: by cold Formylation of Rhodinol ex Geranium.

103-86; 106-317; 163-68; 163-236;

## 2804: RHODINYL PHENYLACETATE

For composition: see monograph: Rhodinol.

Very pale straw-colored, viscous liquid. B.P. approximately 340° C. Sp.Gr. approximately 0.98.

Insoluble in water, soluble in alcohol and oils.

Sweet and very "deep", soft, honey-like Rose fragrance with considerable resemblance to the "fond" of Rose absolute.

Very sweet, Rose-honey-like taste in concentrations below 10 ppm.

This ester is indeed ideal for the foundation of a Rose base. According to the cost permissible, it could be used in concentrations from a few percent to 15 or 25% of the Rose base.

Since Citronellyl phenylacetate has often been marketed under the above label (title material), it would be wise to compare the odor of the two before further experimenting. The cost difference is enormous. And the odor difference may not always be so enormous, except in cases where a true Rose absolute type base is required.

The "true" ester is an excellent fixative, and its rosy or its honey-like character can be emphasized according to the additives of more volatile type. With Sandalwood oil or Santalol, it forms an almost classical background for Oriental-Chypre types, while in general it can be used to supply "richness" to many types of floral fragrance.

Traces of this ester are used in various fruit flavor compositions, imitation Honey, Peach, etc. The concentration in finished products is usually less than 10 ppm, often near 1 ppm.

G.R.A.S. F.E.M.A. No.2985.

Prod.: The production via Phenylacetic acid and Rhodinol (ex Geranium oil) by azeotropic esterification gives a more complete product than the alcohol interchange esterification (via Rhodinol plus Methyl phenylacetate). The two methods, and variations of same, have been used in the manufacture of the title ester.

34-248; 103-141; 106-318; 163-68; 163-236; See also monograph: Citronellyl phenylacetate.

## 2805: RHODINYL PROPIONATE

For composition: see monograph Rhodinol.

Colorless oily liquid. B.P. approximately 255° C. Sp.Gr. approximately 0.91.

Almost insoluble in water, soluble in alcohol and oils.

Rich and sweet, fruity-floral Rose-Geranium type with a fresh, almost Verbena-like undertone and good tenacity. There is an overall balsamic character to this odor which makes it attractive, but also makes it rather unconspicuous.

The title ester is occasionally used as a modifier for the Acetate in Rose, Carnation, Oriental or balsamic fragrance types. It has a richer odor than the Acetate, but it also lacks the freshness of that material. Its sweetness blends very well with balsamic and Citrus-balsamic notes for rich Oriental types.

The ester finds a little use in flavor compositions, e. g. in imitation Plum, Honey, various Berry-compositions and Rose flavors. Its taste is sweet and deep, while Citronellyl propionate is not nearly as sweet or rich. The concentration used in normally about 1 to 5 ppm in the finished product.

G.R.A.S. F.E.M.A. No.2986.

Prod.: from Rhodinol (ex Geranium oil) and Propionic anhydride.

33-622; 103-109; 163-68; 163-236;

## 2806: RHODINYL SALICYLATE

Composition, see monograph: Rhodinol.

Almost colorless, viscous liquid.
Sp.Gr. approximately 1.00.

Practically insoluble in water, soluble in alcohol and oils.

Very weak, sweet-rosy, powdery-balsamic odor of excellent tenacity.

The effect of this ester does not correspond to its very high cost of production. It would be reasonable to test related materials before this material is used, if it is at all available.

The odor type is quite pleasant, but not unusual, while the odor value is very limited. Only the fixative effect is excellent, but not truly worth the price.

If a material corresponding to the title name is still available, it must be quite rare, and the author has the impression that the title ester is obsolete in perfumery.

## 2807: RHODINYL-n-VALERATE

Rhodinyl pentanoate.
Rhodinyl valerianate.
For composition, see: Rhodinol.

Colorless oily liquid. B.P. approximately 274° C. Sp.Gr. approximately 0.91.

Practically insoluble in water, soluble in alcohol and oils.

Heavy-fruity, slightly earthy-green, but also sweet, rosy odor of good tenacity.

The title ester, by some perfumers preferred over the *iso*-Valerate (see next monograph), has found a little use in perfume compositions, mainly of the "Oriental" and Oriental Rose types. Its depth makes it suitable for "red rose" compositions, and its warm-earthy character blends very well with Oakmoss and Vetiver in a Chypre.

It is also an excellent fixative for the terminal notes of Bergamot (likewise in Chypre), and it will support "tabac" notes in an attractive manner.

The material is very rarely offered commercially, but most often manufactured on a small scale by the manufacturers of Rhodinol, for "captive" use by the perfumers in the manufacturing house.

Prod.: from Rhodinol and Valeric acid, by azeotropic esterification.

33-933; 163-68; 163-236;
See also Rhodinyl-*iso*-valerate, next monograph.

## 2808: RHODINYL-iso-VALEARTE

Rhodinyl-*beta*-methylbutyrate.
Rhodinyl-*iso*-valerianate.
For composition, see monograph: Rhodinol.

Colorless oily liquid. B.P. approximately 270° C. Sp.Gr. approximately 0.91.

Practically insoluble in water, soluble in alcohol and oils.

Heavy-rosy, intensely fruity odor of good tenacity. Overall more fruity, but less natural-rosy than the *n*-Valerate.

Again, as with the Butyrate-*iso*-Butyrate, the *iso*-Valerate seems to be preferred by the flavorist, while the *n*-Valerate is preferred by the perfumers. None of the two materials are commonly available. They are only occasionally offered commercially, or manufactured "on order" by the user himself.

The title ester has a relatively refreshing, very sweet, rosy-woody taste in concentrations lower than 10 ppm. It is occasionally used in tobacco flavoring (some customers are willing to pay very high prices for exceptionally good tobacco flavors, and the manufacturer may be able to use Bulgarian Rose oil and similar luxury items in the flavor). Trace amounts are used in various fruit imitation flavors, berry compositions and Rose flavor for carbonated beverages.

The normal concentration in the finished product will be about 2 to 7 ppm.

G.R.A.S. F.E.M.A. No.2987.

(The *n*-Valerate is not specifically mentioned in the American G.R.A.S. list).

Prod.: by azeotropic esterification of Rhodinol with *iso*-Valeric acid.

36-482; 103-125;

## 2809: ROSE OXIDE

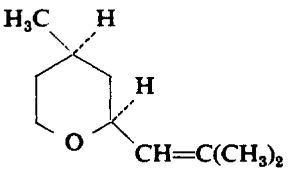
The name "Rose oxide" was originally applied to a hitherto unknown material, isolated in 1959 from Bulgarian Rose oil.

It appears that the oil contained at least two stereo-isomerides of this formula.

The first synthetic "Rose oxide" was a mixture of several isomers, and to-day, ten years later, a pure, single isomer is still a rare material.

The author has preferred to use the name "Rose oxide" rather than the individual, chemically correct names of the isomers.

*cis-2-(2'*-Methyl-*1'*-propenyl)-*4*-methyltetrahydropyran. (Preferred isomer).
The *laevo-cis-* and the *laevo-trans*-forms may be either synthetic or natural.
The *dextro-cis-* and the *dextro-trans*-forms are exclusively synthetic.



Rose oxide "A", also called
Rose oxide "L", $C_{10}H_{18}O = 154.25$
or *cis*-isomer.

Colorless mobile liquid. Sp.Gr. 0.87.
B.P. 182° C. These figures may vary slightly, since commercial "Rose oxides" differ in composition.

Very slightly soluble in water, soluble in alcohol and oils.

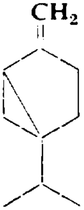
Penetrating and very diffusive, gassy-green or "hard" green, floral odor of poor tenacity. The resemblance to Geranium appears only upon dilution of the Rose oxide, and best in a composition. The diluted material has also a Rose-like character. Certain materials have a less gassy, more "bread-like" topnote, which is warmer and more pleasant than the "gassy" type of odor.

The odor of the *laevo*-isomer is sweeter, yet somewhat green. The odor of the *dextro*-isomer is more warm-spicy, sometimes gassy, more often just herbaceous.

Since Rose oxide is synthesized by quite different ways, the commercial products may contain by-products in various proportions.

# 2810: SABINENE

A monoterpene, naturally occurring in *dextro*- and *laevo*-forms.



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. Sp.Gr. 0.84.
B.P. 165° C.

Insoluble in water, soluble in alcohol and oils.

Warm, oily-peppery, woody-herbaceous and spicy odor of moderate to poor tenacity.

Warm-spicy taste with slightly pungent mouthfeel at concentrations above 50 ppm. Woody-peppery at lower concentrations.

This terpene, although rarely offered commercially, has been suggested for use in various artificial essential oils, mainly Black Pepper oil. It has also been suggested for use in imitation Blackcurrant flavor, a notoriously difficult flavor problem.

The author is not aware of any significant use of the title material as such in perfume compositions. It has not been included yet in the G.R.A.S. list in the U.S.A. In spite of repeatedly published statements that Savin oil (which contains small amounts of this terpene) is relatively toxic, there seems to be a lack of solid evidence about this toxic effect of the oil. Reports indicate that it took 3 grams of Savin oil to kill a Guinea pig, and such high doses place the oil in a relatively low-toxic class of materials. Other reports indicate some very specific and hazardous effects of the oil upon the human systems.

Since the title terpene is present in commonly used materials at much higher concentration than it is in Savin oil, one should assume that the Sabinene is not the hazardous element of Savin oil.

Prod.:

1) by isolation from various essential oils: Cubeb oil (*dextro*-Sabinene), Chamaecyparis obtusa oil (*dextro*-Sabinene), Carrot seed oil (*laevo*-Sabinene).

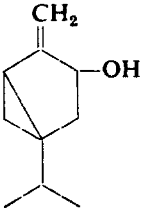
   The Japanese Hiba oil (from Thujopsis dolobrata), particularly the leaf oil, is very rich in Sabinene (40-50%).

2) There is no useful synthesis for this terpene.

7-148; 87-114; 158-217; 85-103; 65-64;

# 2811: SABINOL

*4*-Methylene-*1*-*iso*-propylbicyclo-(*0,1,3*)-hexanol-*5*.
A bicyclic monoterpenoid alcohol.
This monograph refers to *dextro*-Sabinol, which is natural Sabinol.



$C_{10}H_{16}O = 152.24$

This influences the odor greatly, and it may be difficult to substitute a Rose oxide from one manufacturer with that from another – in an already established formula.

Although not even 10 years old as a commercial article, Rose oxide is already a very important perfume chemical (or "material"). Its use in artificial Geranium and Rose oils will immediately represent a sizeable annual consumption by certain large soap manufacturers, while perfumers continue to find new uses for Rose oxide – in fragrances other than Rose, Geranium, etc. Its stability in soap, and its power compensates easily for its cost which is now at a very attractive level (about 3-4 times the price of Geranium oil). Concentrations of 0.1% may have a perceptible "lifting" effect upon a fragrance, not necessarily a rose type. Artificial Rose oils may contain from 0.3% up to more than 1% of Rose oxide, depending upon the type of Rose oxide used.

Artificial Geranium oils will usually contain more than 1%, but less than 3% Rose oxide. Higher concentrations will normally only occur in specialties or bases.

There is not yet any well-defined statement as to which combination of Rose oxide is "the best". The choice is still very subjective, and certain methods of synthesis brings very low-cost Rose oxides to the perfumer. There are cases where a low-cost Rose oxide is of definite advantage, even if it does not carry the true-to-Nature beauty of the preferred isomer or isomer-mixture. As a "lifting" ingredient, Rose oxide can be used in a very ordinary quality, including by-products otherwise not accepted for Rose or Geranium work.

Prod.: (many methods):

1) a great number of patented syntheses start from Citronellol. One method uses autoxidation, followed by reduction and finally acid catalyzed cyclization.
2) from Crotonaldehyde and Vinylether via Ethoxymethyl dihydropyran. Hydration, followed by reaction with *iso*-Butenyl magnesium bromide leads to Rose oxide.

It should be kept in mind, that Geranium oil contains other, related materials, some of which may have been developed through biosynthesis in the plant. One of these materials is:

*2*-Acetonyl-*4*-methyltetrahydropyran (monograph No. 23) ($C_9H_{16}O_2$).

See also monograph:

*2,2,6*-Trimethyl-*6*-vinyltetrahydropyran, an empirical isomer of Rose oxide, naturally occurring in Geranium oil Reunion.

An isomer of that material,

*2,6,6*-Trimethyl-*2*-vinyltetrahydropyran,

has been identified in distilled Lime oil.

Two related chemicals of interest for artificial Geranium are:

*2*-Methyl-*4*-vinyl-*5*-*iso*-propenyl tetrahydropyran, and

*2*-Methyl-*4*-vinyl-*5*-*iso*-propenylidene tetrahydropyran.

90-709; 90-711; 90-731; 90-744; 156-381; 159-475; 163-375;

Recherches, vol. 14, Dec. 1964, p. 96 (Roure-Bertrand Fils & Justin Dupont, S. A.).

Firmenich patents 1330750 and 3161657 (France and U.S.A.).

Dragoco Bulletin (1967) "Rose oxides L and R".

Firmenich data sheet July 1964.

U.S. patent 3,166,576 (1965), R. L. Markus.

German patent 1.137,730 (1962), Klein, Ohloff and Schenk.

Colorless oily liquid. Sp.Gr. 0.94.
B.P. 213° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, but very pleasant, warm, Ambre-Labdanum-like, woody-balsamic odor of moderate tenacity.

If it were not for lack of power, this would undoubtedly be a very desirable perfume chemical. Considerable research-effort has been concentrated upon Juniperberry oil, Savin oil, Cypress oil during the years to elucidate the problem of identifying olfactorily important component in these oils.

Juniperberry oil has had a "come-back" in perfumery, and there is a marked shortage of the good quality oils. Any material with a similar odor type would be looked upon with great interest from the perfumer and the perfume chemist.

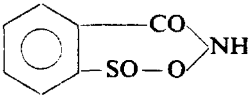
At the time of editing this monograph, the title material is not a common commercial article. It is occasionally prepared by the interested party for private use. With Lavender, Lavandin, Citrus oils, Labdanum, Leather notes, Styrax, etc. it gives very attractive notes for "Men's Fragrances", Colognes, etc. It is also interesting in Chypre types for women, and as a modifier in Ambre types.

Prod.: by isolation from Savin oil, or from certain Orthodon oils in which the alcohol is the chief component. The Sabinol thus isolated is *dextro*-Sabinol.

67-551; 88-209; 95-106; 96-84; 1-707;

## 2812: SACCHARIN

*1,2*-Benz-*iso*-thiazol-*3*-(*2H*)-one-*1,1*-dioxide.
*2,3*-Dihydroxy-*3*-oxobenz-*iso*-sulfonazole.
*ortho*-Benzosulfimide.
*ortho*-Sulfobenzimide.
*1,2*-Dihydro-*2*-ketobenz-*iso*-sulfonazole.
"Gluside" – –
– and a huge number of trade names.



$C_7H_5NO_3S = 183.19$

White crystals or white crystalline powder. M.P. 228° C. (decomposes).

0.35% soluble in water, 3.3% soluble in alcohol, about 1% soluble in many oils. Easily soluble in aqueous alkali.

Odorless. Intensely sweet taste, followed by a less pleasant astringent or metallic, sometimes described as bitter, after-taste, depending on the concentration of Saccharin tasted.

Aqueous solutions break down in boiling water to non-sweetening matter.

The minimum perceptible level of concentration (which is very subjective) is estimated at 2 to 15 ppm. Among the *odorless* materials, it has a relatively powerful taste.

The sweetness of Saccharin is enhanced through the presence of certain other sweeteners, e. g. Dulcin. Although Dulcin is a weaker sweetening agent than Saccharin, a mixture of the two will taste sweeter than the full amount of any single one of the two. However, Dulcin is not permitted for food in the U.S.A.

Combinations of Saccharin with Cyclamates are frequently used in modern "low-calorie" beverages, candy, etc. The normal proportion is one part of Saccharin to 9 parts of Cyclamate. This mixture is more than twice as sweet as the full amount of Cyclamate.

Saccharin is estimated as being 500 to 550 times sweeter than cane sugar.

Saccharin (and Sodium saccharin, see monograph) are deemed G.R.A.S. by the American F.D.A. (Food and Drug Administration).

A "sugar-free" American beverage may (according to its label) contain 80 to 100 ppm of Calcium cyclamate plus 4 to 5 ppm of Saccharin as total sweetening ingredients, but these figures may vary considerably. Since the American authorities are becoming increasingly concerned about the enormous intake of artificial sweeteners by people who are in no way "ill" – in spite of the required labelling "for people who must restrict their intake of sugar", the declarations on beverage labels, candy wrappers, etc. are becoming more and more elaborately clever and confusing.

It would be simple to calculate that in order to achieve sweetening effect equivalent to 10% sugar (average sweetening of carbonated beverages), one would have to use 200 ppm of Saccharin or a mixture of 100 ppm of Saccharin plus 2000 ppm of Calcium cyclamate. Even with an estimated synergistic effect (which is not very pronounced in this case), these figures can not be lowered considerably.

The fact that Saccharin – when compared to a 10% cane sugar solution – is only 330 to 350 times sweeter, would further increase the above figures.

More "true-to-the-fact" figures are available for "dietetic jellies" where the concentration of Saccharin (or Saccharin sodium) is given at 300 to 400 ppm, in combination with 3500 to 4500 ppm of Sodium cyclamate. These figures may vary slightly according to the type of jelly and the acidity of the fruit juice used in the jelly.

The "confusion" may arise from the fact that some manufacturers will indicate that their beverage contains only "xx" calories *per ounce*, and "yy" *parts* of artificial sweetener (name given). The manufacturer may avoid the indication that the sweeteners are present in the amount of "yy parts *per gram*" leaving the customer to believe that it is? – of course – per ounce.

The above remarks may be understood as one example of the confusing situation existing in the interim period until very firm statements are made by the authorities, including absolutely unambiguous and precise limitations for the addition of sweetening agents, formulations of the required statement on the label, and whether or not this product should be reserved for truly "ill" people only.

Otherwise, we may find ourselves faced with the same type of label as known from the American cigarette package: "Caution – (intake of artifically sweetened sodas) may be hazardous to your health". Which leaves it up to the customer to decide about his own health.

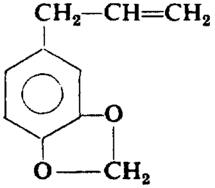
Saccharin is now 90 years old, and it has held up through many and thorough tests and physiological research programs. It is still the major sweetener in most countries, but it was not meant to be part of everybody's everyday life. The "body-weight-watching" fashion is world-wide, and it has caused an enormous increase in the use of artificial sweeteners by people who never really needed it – people who just lack the strength of character to eat less or excercise more – or both.

Prod.: Basically from Toluene, via methods with many variations: e. g. via *ortho*-Toluene sulfonamide, by oxidation with aqeuous Potassium permanganate to *ortho*-Sulfamoyl benzoic acid, which is dedydrated to Saccharin.

1-540; 69-384; 100-914; 159-516; 162-511; B-XXVII-168; private experiments.

## 2813: SAFROLE

*3,4*-Methylene dioxyallylbenzene.
*4*-Allyl-*1,2*-methylenedioxybenzene.
*meta*-Allylpyrocatechin methylene ether.



$C_{10}H_{10}O_2 = 162.19$

Colorless or very pale straw-colored oily liquid. Solidifies in the cold. M.P. 11° C. B.P. 235° C. Sp.Gr. 1.10.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in Propylene glycol and Glycerin.

Sweet and warm-spicy, woody-floral odor of moderate tenacity. To the American public, familiar with Sassafras root, common in the Eastern areas, the odor of Safrole has much in common with that of the root oil, but lacks the rich, creamy sweetness of the root bark oil.

The taste in concentrations below 100 ppm is warm, spicy, but not as "rooty" as that of Sassafras oil.

The use of Safrole in perfumery has always been very small. The three major natural oils (or fractions of oils): North American Sassafras oil, Brazilian Ocotea oil, and Camphor oil fractions, have been preferred in perfumery on account of their lower cost, pleasant odor complex and ready availability. The North American Sassafras oil has slowly decreased and almost vanished from the market in price competition with the two other sources of Safrole-oils.

In the shape of "Camphor oil 1070" or Camphor oil "Sassafrassy", the Camphor oil fractions, rich in Safrole, are extensively used in perfumery for low cost fragrances to the "heavy-duty-cleaning" detergents, floor-cleaners, deodorizing or masking agents for household and industrial purposes, etc. They were also used in "perfuming" of labels and adhesive tapes, in which the glue had an offensive odor (often from decaying glue, or from the phenols used as bactericides against such action). But the use of Safrole in label gum is largely abandoned since the Safrole was banned from use in food flavors.

The Brazilian Ocotea oil, priced almost equal to Camphor oil 1070, is used for the same purposes. The market price in 1968 was only a little more than U.S. $ 1.00 per kilo.

Safrole has been used in flavors for more than half a century, prior to its banning from food flavors according to the American Food and Drug Administration regulation in 1958. Many countries followed the trend and banned the use of Safrole in flavors. However, the use of Safrole in flavors was already "restricted" in the sense that many European countries never had used Safrole in flavors – due to the simple fact that people did not like the taste of Safrole.

This original antipathy may partly have come out of the common psychologigal reaction against a flavor type, if it is already well known for some quite different purpose – such as gummed labels, paper tape, glue, etc. And that is what Safrole was known for in many European countries. The same could be said about Methyl salicylate, which has a very hard time "getting in" on the European candy market – or toothpaste market, while it is a very natural thing in North America.

Safrole was often used in combination with Ginger, Wintergreen (Methyl salicylate), Lemon, Orange, Vanilla, etc. or with Anise (Anethole). The concentration showed great variations, since Safrole, like Anethole, produces an agreeable or acceptable flavor at concentrations ranging from about 20 ppm up to 5000 ppm – in exceptional cases even higher.

In order to maintain consumer products of similar flavor, the use of "Safrole-free" extracts of the root bark of the tree, Sassafras albidum, have been permitted in the U.S.A. These extracts are aqueous extracts and contain no oil portion.

It is interesting to note that the leaves of Sassafras albidum are permitted as a source of food flavor. The leaves have a very pleasant Lemon-Tea-like aroma, without any perceptible trace of the Safrole-type notes in the root bark.

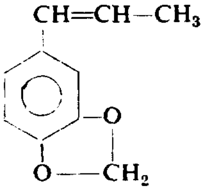
Prod.: Safrole is produced exclusively by isolation from natural oils. The Brazilian Ocotea oil and the Formosan-Japanese-Chinese Camphor oil fractions are the main sources. They contain 70 to 90% Safrole. The need for *iso*-Safrole (from Safrole) for the production of Heliotropine largely determines the price and availability of these oils.

A synthetic process of making Safrole exists, but it is far from being economical: Catechol methylene ether is reacted with Allyl chloride, or 4-Allyl catechol is reacted with Methylene iodide.

1-440; 65-526; 68-974; 72-81; 85-103; 90-449; 95-122; 96-104; 100-915; 103-169; 104-115; 104-461; 104-580; 106-320; 140-171; 159-466; 162-711; 163-69; 163-237; 163-375; B-XIX-39; Am. Perf. 1958, Jan., page 57ff.

## 2814: iso-**SAFROLE**

*4*-Propenylcatechol methylene ether.
*1,2*-Methylenedioxy-*4*-propylene benzene.
*3,4*-Methylenedioxy propylene benzene.
*4*-Propylene-*1,2*-methylenedioxy benzene.
Two diastereoisomerides are known:
The *cis*-form is unstable.
The *trans*- or *beta*-form is the common one.



$C_{10}H_{10}O_2 = 162.19$

Colorless oily liquid. Solidifies in the cold. M.P. 7° C. B.P. 248° C. (*trans*-).

Insoluble in water, poorly soluble in Propylene glycol and Glycerin, soluble in alcohol and oils.

Warm and sweet, soft, floral-anisic, mildly spicy and tenacious odor. Sweeter, more floral, more anisic, less woody-spicy than Safrole.

Sweet, warm, mostly floral taste in concentrations near 30 ppm. Tends to appear perfumey at higher concentrations.

The title material is very well known by name, but hardly ever used as such in perfumery. It serves as an intermediate in the manufacture of Heliotropine, although certain methods avoid this step altogether.

*iso*-Safrole is not permitted in flavors in the U.S.A., and also banned from food flavors in most other countries.

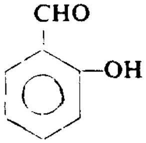
The odor type of *iso*-Safrole is not particularly desirable in perfumery, and the material tends to polymerize upon standing. Such disadvantages make the product vanish from the shelves of perfume laboratories, and it can be considered as very rare or almost obsolete as a perfume or flavor material – as such.

Prod.: from Safrole by treatment with Potassium or Sodium hydroxide in dry state or alcoholic solution, under pressure or at atmospheric pressure.

65-529; 68-977; 72-86; 90-456; 95-123; 96-104; 100-581; 106-214; 156-177; B-XIX-35;

## 2815: SALICYLIC ALDEHYDE

*ortho*-Hydroxybenzaldehyde.
Salicylaldehyde.



$C_7H_6O_2 = 122.13$

Colorless mobile liquid. Solidifies in the cold. M.P. 2° C. B.P. 196° C. Sp.Gr. 1.17.

Slightly soluble in water, miscible with alcohol and oils.

Pungent, irritating odor reminiscent of Benzaldehyde, Acetophenone and Nitrobenzene, but with distinct halogeno-phenolic notes. The author agrees with the late Mr. E.S. Maurer (103-298) that the common description "pleasant floral New-Mown-Hay odor" is not only misleading, but also very incomplete. Even if the odor would be generally described as "pleasant and floral", one should avoid phrases which almost imply or encourage a use of a hazardous material.

In extreme dilution, the odor is warm, herbaceous, spicy-floral but the phenolic note remains perceptible.

It may be a surprise to the perfumer, that the material is used in flavors. The taste in concentrations below 10 ppm is Nut-like, vaguely Coumarin-like/caramellic, warm, slightly spicy.

Since it is generally agreed, that Salicylic aldehyde represents a hazard to human skin, the use of this material in perfumes has been practically abandoned. The aldehyde is occasionally used in technical perfumery, in masking odors for technical purposes, etc. There is no authoritative regulation against the use of Salicylic aldehyde in perfumes, but the "ban" is entirely a voluntary one, a matter of precaution.

The title material is used in imitation Butter, Caramel, Nut, Cinnamon, fruit and spice blends, Muscatel flavor, Violet imitation flavor, etc. in amounts equivalent to 0.5 to 6 ppm in the finished product. Concentrations up to 20 ppm can be found in chewing gum.

The relative tolerance with respect to toxicity of Salicylic aldehyde as compared to Nitrobenzene and Salicylic acid is: 144/100/182 – or, in plain words, the aldehyde is more than half as toxic as Nitrobenzene and it is more toxic than Salicylic acid.

While sensible human laws agree that a human being is "innocent until proven guilty", the author feels that the reverse viewpoint upon flavor materials would help reconstitute the public feeling of safety in foods, e. g. by using the "prevention is better than cure" or "safety first" ideology. A complete ban on the use of materials such as Salicylic aldehyde, until solid proof of harmlessness is published, would be very comforting.

The alternative would be a proof that certain, specified, low levels of concentration of the material, are harmless to human beings.

G.R.A.S. F.E.M.A. No.3004.

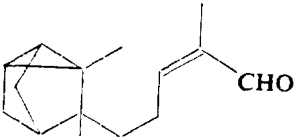
Prod.:

1) the original synthesis used Sodium phenolate and Chloroform, heated with Potassium hydroxide.
2) More modern methods use esters of *ortho*-Cresol, e. g. *ortho*-Cresyl carbonate or Tri-*ortho*-cresyl phosphate (TCP) and proceed via chlorination and saponification to Salicylic aldehyde.

31-61; 68-741; 85-104; 90-494; 100-916; 103-298; 140-162; 159-410; 163-237; 95-140; 96-123; B-VIII-31; 1-512;

## 2816: SANTALAL

Santal aldehyde.
*alpha*-Santalal.



$C_{15}H_{22}O = 218.34$

Colorless, slightly viscous liquid.
B.P. 265° C. Sp.Gr. 1.00.

Insoluble in water, soluble in alcohol and oils.

This tricyclic sesquiterpenaldehyde, corresponding to the alcohol Santalol, is known in its *alpha*-form.

It has a refreshingly sweet-woody, very tenacious odor, by some observers considered superior to that of Santalol, at least with respect to strength. It is doubtful whether the pure material has yet been prepared, and it is apparently not commercially available.

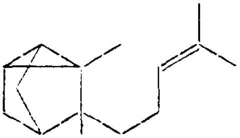
The material is briefly mentioned here in support of the rather meager information so far available on the subject of artificial Sandalwood odors (chemicals) of similar structure, but not of natural origin.

Prod.: by chromic acid oxidation of *alpha*-Santalol.

A partial synthesis has also been elaborated.

67-646; 67-673; 87-328; 89-125;

## 2817: alpha-SANTALENE



$C_{15}H_{24} = 204.37$

Colorless oily liquid. B.P. 253° C.
Sp.Gr. 0.91.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet-woody odor of excellent tenacity. The odor is generally considered superior to that of *beta*-Santalene (see next monograph).

This tricyclic sesquiterpene is probably not widely used as such in perfumes (or flavors), but it serves a purpose in its natural state as part of the Sandalwood oil picture.

It would therefore be of potential interest as an additive to some of the newer Sandalwood-smelling chemicals, in which there is a general lack of "oily"-woody sweetness, presumably deriving from components other than the Santalols.

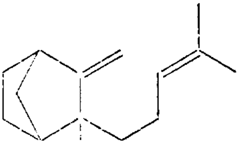
The title material is included here as an example of a Sandalwood-smelling chemical. It is rarely available in the pure state as it is extremely difficult to separate it from the accompanying *beta*-Santalene.

Prod.:

1) by isolation from East Indian Sandalwood oil.
2) synthetic from Camphor via *alpha*-Bromocamphor and its Grignard derivative to the title material.

67-645; 87-325; 95-78; 96-56; 163-375;

## **2818:** beta-**SANTALENE**



$C_{15}H_{24} = 204.37$

Colorless oily liquid. B.P. 264° C.
Sp.Gr. 0.89.

Insoluble in water, soluble in alcohol and oils.

Mild, woody odor, more dry, less sweet than the odor of the *alpha*-Santalene (see previous monograph). The tenacity is excellent, but most observers find the odor type inferior and undesirable.

This bicyclic sesquiterpene is rarely commercially available. There is no real interest in having the isolated material, other than the academic interest for the study of Sandalwood odors and chemical structure. The material is included in this work for the sake of completing the description of chemicals, related to Santalol, and at one time commercially available or presumed to be of olfactory value.

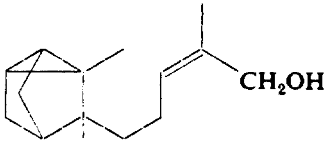
Prod.:

1) by isolation from saponified East Indian Sandalwood oil. It is extremely difficult to separate the *alpha*- and *beta*-Santalenes by fractional distillation.
2) a Synthesis starting from Isoprene and *beta*-Phellandrene has been suggested but it has no commercial importance.

67-646; 87-327; 95-78; 96-56;

## **2819:** alpha-**SANTALOL**

"Argeol".
"Arheol".
*dextro-alpha*-Santalol.



$C_{15}H_{24}O = 220.36$

Almost colorless, viscous liquid. B.P. 302° C.
Sp.Gr. 0.98.

Practically insoluble in water, soluble in alcohol and oils, poorly soluble in Propylene glycol and Glycerin.

Sweet and very rich, warm-woody, tenacious odor. Santalol is generally considered to be a refined edition of the Sandalwood oil odor. Free from the slightly nauseating-gassy, sometimes green-woody, rather pungent and less delicate notes. *alpha*-Santalol is considered the desirable odor type of the two, although the two isomers (*alpha*- and *beta*-) are rarely offered individually in the pure state.

The title tricyclic sesquiterpene alcohol is frequently used in perfume compositions, not only in the classical "Oriental" types, but in many modern-woody fragrances, Chypre variations, Muguet undertones and fixateur, Carnation, etc. It blends excellently with many resins and balsams, Opopanax, Myrrh, Tolu and Peru, with Geranium, Patchouli, Ionones, Methylionones, Vetiver, etc.

Cyclamen aldehyde performs interestingly over the Santalol base, and the musks support the sweet-woody notes very well.

Santalol is also used in flavor compositions, in trace amounts in various floral and fruity complexes. The concentration will rarely exceed 10 ppm in the finished product. Santalol shows less tendency of "standing out" of a flavor than does Sandalwood oil. It is, in other words, much easier to use Santalol in a flavor than it is to use Sandalwood oil.

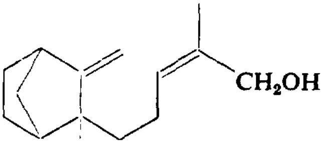
G.R.A.S. F.E.M.A. No.3006 (as "Santalol", *alpha-* and *beta*).

Prod.: by isolation from East Indian, West Australian or Timor type Sandalwood oils. The commercial product, Santalol, consists of a mixture of *alpha-* and *beta*-Santalol, with a preponderance of the *alpha*-isomer.

67-672; 85-105; 88-332; 95-107; 96-87; 100-919; 106-322; 163-69; 163-237; 65-266;

## 2820: beta-SANTALOL

*laevo-beta*-Santalol.
A bicyclic sesquiterpene alcohol.



$C_{15}H_{24}O = 220.36$

Almost colorless, viscous liquid. Sp.Gr. 0.98. B.P. 309° C.

Insoluble in water, soluble in alcohol and oils.

Sweet, woody and very tenacious odor.

The commercial product "Santalol" is the mixture of *alpha*-Santalol and *beta*-Santalol, obtained by isolation from Sandalwood oil. The two Santalols are rarely available as individual materials, although perfumers have at times expressed preference for the *alpha*-isomer. The author believes that it would take further work and distinct isolation, odor-evaluation, etc. of the two isomers, before any definite statement could be made. The fact that the *alpha*-Santalol preponderates in the natural oil may not be any supporting proof that it is also the better smelling isomer.

The American authorities have covered this problem temporarily by declaring both *alpha-* and *beta*-Santalol G.R.A.S., and listed the material as "Santalol" (*alpha-* and *beta*).

It is interesting, however, that the research chemist offers a suggested synthesis for *beta*-Santalol, while there is more doubt about a possible synthesis for the *alpha*-isomer.

See also general comments under monograph: *alpha*-Santalol.

G.R.A.S. F.E.M.A. No.3006 (as "Santalol").

Prod.:

1) *beta*-Santalol comes as a minor component of "Santalol", obtained as an isolate from Sandalwood oil. The separation of the two isomers by fractionated vacuum distillation is very difficult, if not nearly impossible. It may be necessary to produce derivatives of the two isomers in order to separate them quantitatively. The separation has no commercial interest.
2) A synthesis starting from *3*-Methyl-norcamphor-*3*-bromopropionate has been suggested, but it has no commercial importance.

65-208; 67-672; 85-105; 88-34; 95-107; 96-87; 100-919; 106-322; 163-69;

## 2821: SANTALYL ACETATE

The commercial product is a mixture of *alpha-* and *beta*-Santalyl acetates.
Structure, see monograph: Santalol.

$C_{15}H_{23}—OOC—CH_3$

$C_{17}H_{26}O_2 = 262.40$

Almost colorless or very pale straw-colored, slightly viscous liquid. Insoluble in water, soluble in alcohol and oils. B.P. 315° C.
Sp.Gr. 0.99.

Delicately woody, faintly Sandalwood-like, musky-sweet odor of excellent tenacity. The absence of the "medicinal" notes of Sandalwood is characteristic of this ester.

Santalyl acetate comes on the market in a variety of qualities. Some products seem to be undestilled Acetylation-products of the whole oil, while others are highly refined esters, made from the isolated alcohols of Sandalwood. There are qualities "inbetween" these, too. Similar observations are made with the Acetates from Guaiacwood, Vetiver, Amyris, etc.

The title ester finds some use in perfume compositions for Chypres, Oriental-woody fragrances (in support of the Sandalwood odor), variations of Lilac and other mild florals, etc. It is an excellent fixative.

It is also used in flavor compositions as a trace component in imitation Apricot, Pear, Peach, Pineapple, floral flavor types, etc.

The concentration used is normally equivalent to about 0.5 to 2 ppm in the functional product.

Two esters of Santalol are permitted in food flavors in the U.S.A.: the other is Santalyl phenylacetate.

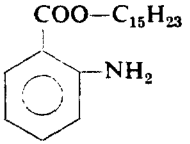
G.R.A.S. F.E.M.A. No.3007.

Prod.: by Acetylation of Santalol.

33-504; 36-484; 103-100; 106-324; 163-69; 163-237;

## 2822: SANTALYL ANTHRANILATE

Santalyl-*ortho*-aminobenzoate.
The commercial product, when available, is not pure ester. The ester portion is furthermore a mixture of *alpha-* and *beta*-Santalyl anthranilates.
Structure – see monograph: Santalol.



$C_{22}H_{29}NO_2 = 339.48$

Pale straw-colored, viscous liquid.
B.P. over 330° C.

Practically insoluble in water, soluble in alcohol and oils.

Although there are materials of very different olfactory quality on the market, the desirable type has a very delicate, fine, floral and sweet-tenacious odor, more floral than woody, and with practically no trace of Sandalwood-oil-odor.

The title ester is occasionally offered commercially, but it has generally failed to interest the perfumer, and it may be considered as almost obsolete in perfumery today. Its odor "value" is very low, and its cost unreasonably high. It is included in this work mainly to complete the description of Santalyl esters available, or formerly available.

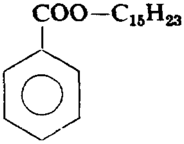
As a fixative in delicate florals, it has excellent effect, but the perfumer has a number of better suggestions on his shelf today, at a much lower cost.

Prod.:
1) from Santalol and Isatoic anhydride.
2) from Santalol and Methylanthranilate.

61-74;

## 2823: SANTALYL BENZOATE

A mixture of
*alpha-* and *beta*-Santalyl benzoates.
Complete structure - see monograph: Santalol.



$C_{22}H_{28}O_2 = 324.47$

Almost colorless, viscous liquid. B.P. 345° C. Sp.Gr. 1.00.

Insoluble in water, soluble in alcohol and oils.

Very faint, balsamic, delicately woody-floral odor of excellent tenacity.

The title ester has once been available, but the author finds that it is of very little interest to the perfumer, and it can be considered as practically obsolete.

It is an excellent fixative, but its contribution of odor is very small compared to the relatively high cost of this material. It can easily be replaced by very effective and less expensive modern fixatives, while its odor type can be imitated with additional, new materials.

Prod.:
1) from Santalol and Methylbenzoate.
2) from Santalol and Benzoic acid by azeotropic esterification.

163-69;

## 2824: SANTALYL-n-BUTYRATE

A mixture of *alpha-* and *beta*-Santalyl-*n*-butyrates.
Structure - see monograph: Santalol.

$C_{15}H_{23}—OOC—CH_2—CH_2—CH_3$

$C_{19}H_{30}O_2 = 290.45$

Practically colorless, slightly viscous liquid. B.P. 320° C. Sp.Gr. 0.97.

Insoluble in water, soluble in alcohol and oils.

Balsamic-fruity, heavy and tenacious, woody Tearose type of odor.

This ester finds a little use in perfume compositions. It is very suitable for classical Chypre types, "tabac" notes and powder perfumes, where its warmth and great tenacity are welcome. "Oriental" rose bases and "tabac-rose" types may include this material in its undertones and fixative portion. It blends very well with the Phenylacetates and Civet, Styrax, Castoreum, Patchouli, etc. for heavy floral-balsamic fragrances.

Prod.: by azeotropic esterification of Santalol with *n*-Butyric acid.

33-733; 103-117; 163-70; 163-237;

## 2825: SANTALYL-iso-BUTYRATE

A mixture of *alpha-* and *beta*-Santalyl-*iso*-butyrates.
Structure - see monograph: Santalol.

$C_{15}H_{23}—OOC—CH(CH_3)_2$

$C_{19}H_{30}O_2 = 290.45$

Almost colorless, slightly viscous liquid. Sp.Gr. 0.97. B.P. 316° C.

Insoluble in water, soluble in alcohol and oils.

Fruity-balsamic, sweet and woody, very tenacious odor, not as mellow or "round" as the odor of the *n*-Butyrate, but slightly fresher.

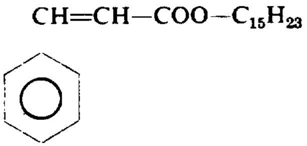
This ester, by most perfumers considered less interesting than the *n*-Butyrate, but by many chemists considered less prone to decompose and produce free acid, is occasionally used in perfume compositions of the Chypre, Fougère, Moss-rose, "tabac", Bruyère and similar fragrance types. It supplies excellent fixation in a Fougère, and it may contribute to the most desirable notes in a powder perfume. It is also a common ingredient in the rather unfashionable type of fragrance, called "Oriental Rose".

Prod.: by azeotropic esterification of Santalol with *iso*-Butyric acid.

33-734; 155-128; 163-70;

## 2826: SANTALYL CINNAMATE

A mixture of *alpha-* and *beta*-Santalyl cinnamates.
Structure – see monograph: Santalol.



$C_{24}H_{30}O_2 = 350.50$

Very pale straw-colored, viscous liquid.
B.P. over 330° C.

Insoluble in water, soluble in alcohol and oils.

Very fine, but faint, floral-balsamic odor of excellent tenacity.

Although suggested as a base or undertone material for Muguet or other delicate floral bases, this ester has found very little use in perfumery. Its greatest asset is that of being an excellent fixateur, but its cost is prohibitive for such purpose, except in rare types of luxury perfumes. Even so, its effect can be duplicated with more modern and well-defined, available materials at much lower cost.

The ester can be considered as almost obsolete in perfumery.

Prod.: from Santalol and Methylcinnamate, or by azeotropic esterification of Santalol and Cinnamic acid, using a Sodium naphthalenesulfonate type catalyst.

61-75;

## 2827: SANTALYL FORMATE

The commercial material is a mixture of *alpha-* and *beta*-Santalyl formates.
Structure – see monograph: Santalol.

$C_{15}H_{23}$—OOCH

$C_{16}H_{24}O_2 = 248.37$

Colorless, slightly viscous liquid.
B.P. 290° C. Sp.Gr. 1.00.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-ethereal-floral, also herbal, Sandalwood odor, without the "medicinal" character of the natural oil, yet more woody and dry. Good tenacity.

This ester, very rarely available commercially, has been suggested for use in perfume compositions.

As supporting note for Santalol, as undertone in Cassie and Mimosa variations, in Chypre and Oriental fragrances (it blends very well with Geranium oil), it could find some use.

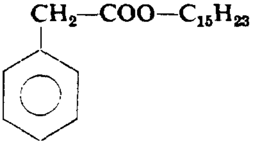
However, it is very difficult to obtain in a satisfactory quality, and the material is generally missing in a perfume laboratory, and is inknown to many perfumers.

Prod.: by cold formylation of Santalol.

33-412; 36-484; 103-87; 163-70;

## 2828: SANTALYL PHENYLACETATE

Santalyl-*alpha*-toluate.
A mixture of *alpha*- and *beta*-Santalyl phenylacetates.
Complete structure – see monograph: Santalol.



$C_{23}H_{30}O_2 = 338.49$

Almost colorless or very pale straw-colored, viscous liquid. B.P. 328° C. Sp.Gr. 1.02.

Insoluble in water, soluble in alcohol and oils.

Very heavy, musky-rosy, waxy or honey-like, sweet and very tenacious odor. There are considerable variations in the odor of materials from different manufacturers. This is a rather typical feature of Phenylacetates of "heavy" alcohols.

The title material, probably the second-most important ester of Santalol next to the Acetate, is used in perfume compositions for its outstanding fixative value, its ability to blend with floral, balsamic, mossy, Ambre-like, Oriental or musky fragrance types, and its good stability (provided it is a good quality ester).

It blends very well with the resins and balsams, with Rose and Labdanum, tabac or "animal notes", etc.

The title material is also used in flavor compositions for imitation Caramel, Honey, Butter, for fruit complexes, etc., mostly as a fixative. The concentration in the finished product will normally be about 1 to 2 ppm.

G.R.A.S. F.E.M.A. No.3008.

Prod.: from Phenylacetyl chloride and Santalol.

It has also been prepared from Methyl-phenylacetate and Santalol, and by azeotropic esterification of Santalol with Phenylacetic acid in presence of a catalyst.

34-248; 36-484; 106-326; 163-70; 163-237;

## 2829: SANTALYL PROPIONATE

A mixture of *alpha*- and *beta*-Santalyl propionates.
Structure – see monograph: Santalol.

$C_{15}H_{23}—OOC—CH_2—CH_3$

$C_{18}H_{28}O_2 = 276.42$

Almost colorless, slightly viscous liquid.
B.P. 318° C. Sp.Gr. 0.98.

Insoluble in water, soluble in alcohol and oils.

Mild and delicately fruity-woody, tenacious odor, free from the "medicinal" character of Sandalwood oil. Milder and rounder (mellower) than the Acetate.

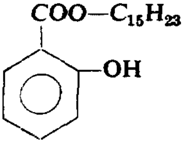
Apart from being a pleasant variation of the Acetate, this ester has very little to offer the perfumer. It may find some use in exotic or floral bases, or it may support the delicately woody undertones in a Muguet or Chypre, but it is generally unknown and very rarely offered commercially.

Prod.: by azeotropic esterification of Santalol with Propionic acid. It has also been prepared from Santalol with Propionic anhydride.

36-484; 163-70;

## 2830: SANTALYL SALICYLATE

Santalyl-*ortho*-hydroxybenzoate.
A mixture of *alpha*- and *beta*-Santalyl salicylates.
For complete structure – see monograph: Santalol.



$C_{22}H_{28}O_3 = 340.47$

Yellowish oily liquid. Sp.Gr. 1.07.
B.P. over 320° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, sweet-balsamic-woody odor of excellent tenacity.

The title material has had some application in pharmaceutical praxis, but the author is not aware of any use of the ester in perfumery, except in rare cases as a fixative.

It has been included in this work for the sake of completing the description of the Santalyl esters, also such esters which have only briefly had any application in perfumery.

The effects derived from the title ester can easily be duplicated at a lower cost with more modern and well-defined, available materials, and it is reasonable to assume that the material is practically obsolete in perfumery.

Prod.:
1) from Santalol and Methylsalicylate.
2) by azeotropic esterification of Santalol and Salicylic acid in presence of a catalyst.

100-919; 163-237;

## 2831: SANTALYL-n-VALERATE

Santalyl-*n*-pentanoate.
A mixture of *alpha*- and *beta*-Santalyl-*n*-valerates.
Structure – see monograph: Santalol.

$C_{15}H_{23}—OOC(CH_2)_3CH_3$

$C_{20}H_{32}O_2 = 304.48$

Almost colorless, slightly viscous liquid.
B.P. 324° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

Heavy-fruity, delicately woody-herbaceous odor of excellent tenacity.

This ester is very rarely offered commercially, and its use in perfumery is very limited. Occasionally, its fixative value and delicate blend of sweet-woody and root-like, herbaceous notes are utilized in a Chypre or "tabac" type fragrance.

The ester is occasionally used in imitation Apple flavor as a fixative, but even for this purpose, the material is practically obsolete.

Prod.: by azeotropic esterification of Santalol with *n*-Valeric acid.

163-70;

## 2832: SANTALYL-iso-VALERATE

Santalyl-*beta*-methylbutyrate.
A mixture of *alpha*-Santalyl-*iso*-valerate and *beta*-Santalyl-*iso*-valerate.
Structure – see monograph: Santalol.

$C_{15}H_{23}—OOC—CH_2—CH(CH_3)_2$

$C_{20}H_{32}O_2 = 304.48$

Almost colorless, slightly viscous liquid.
B.P. 320° C. Sp.Gr. 0.96.

Insoluble in water, soluble in alcohol and oils.

Fruity-rosy, peppery-woody, delicate and tenacious odor.

Although there is a marked difference between the odor of the title material and that of the *n*-valerate, there is very little interest in this material. Its tenacity is an advantage, but it comes at high cost, and it is not accompanied by any very unusual fragrance notes.

It is interesting that the title material is less Apple-like than the *n*-Valerate (previous monograph), but apparently the two materials have found only little use in flavor compositions.

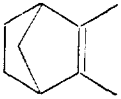
The title material is occasionally used in "tabac" and Bruyère type fragrances, mainly as a fixative for rosy or sweet-woody notes.

Prod.: by azeotropic esterification of Santalol with *iso*-Valeric acid.

36-484; 163-237;

## 2833: SANTENE

*2,3*-Dimethylbicyclo- (*1,2,2*)-heptene-*2*.
A hydrocarbon, resembling the Monoterpenes, but not a terpene in the original meaning of the term.



$C_9H_{14} = 122.21$

Colorless, mobile liquid. B.P. 140° C.
Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Ethereal-gassy, sweet-camphoraceous odor, in high concentration rather unpleasant, but upon dilution sweeter, less gassy, more Camphene-like, balsamic. Poor tenacity.

The material tends to polymerize, become viscous and odorless.

Apart from experimental use in artificial Sandalwood oil, as a minor component with Sandela-type chemicals, this hydrocarbon has not yet found much use in perfumery.

Its presence in Sandalwood oil has led to believe that it forms part of the Sandalwood odor picture, which is true to a certain degree, but it is quite possible that the material, if made available at an attractive, low cost, could be used in volume in Pine needle type fragrances for household products, etc., where low tenacity and diffusive odor is sometimes desirable.

The material is not regularly available on a large scale.

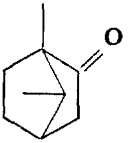
Prod.:

1) by isolation from Sandalwood oil or from various Pine needle oils.
2) synthetic – from Nor-borneol.
3) By dehydration of Camphenilol. This synthesis starts from Camphene via *omega*-Nitrocamphene to Camphenilone, and by hydrogenation to Camphenilol.

67-580; 87-209; 95-68;

## 2834: SANTENONE

*π*-Nor-camphor.
(A lower homologue of Camphor).
Exists in *dextro-* and *laevo*-forms, *dl*-form, and *alpha-* and *beta*-isomers.



$C_9H_{14}O = 138.21$

White or colorless, crystalline mass, or granular crystals. M.P. between 50° C. and 61° C. for the commercially available forms. B.P. about 197° C.

Sweet-camphoraceous, diffusive odor. In dilution quite pleasant, not as "medicinal" as Camphor, not "piney" as Camphene, but rather warm and balsamic.

This ketone is briefly mentioned in the present work, because the material may become an interesting perfumery item, if newer synteses will produce the ketone at an attractive cost. Until then, the material has little more than academic interest.

As a modifier in Lavandin and other herbaceous oils, and as a new material for modern Pine fragrances, it could have interesting possibilities, but it must then be available at much lower cost.

Prod.:

1) by isolation from Sandalwood oil (*laevo*-form only).
2) by oxidation of Santene (see monograph) with Chromic acid.
3) from Camphenilone.
4) by oxidation of Nor-borneol.

67-581; 89-360;

## 2835: SAPONIN

A group or type of Glycosides.

The general structure is a combination of a "sapogenin" which may be a Triterpene or a Steroid, with a "sugar" which may be either Glucose, Galactose, Pentose or Methylpentose.

Hydrolysis will decompose a saponin in the two components.

The saponins used in food and flavor work (little, if any, is used in perfumery) are generally extracted from plant material.

The most common sources are:
Quillaya bark,
Sarsaparilla rhizomes or roots,
Chlorogalum pomeridianum (The California soap plant),
Ginseng (as a by-product).

Other sources are known and used, according to the local availability.

Saponins form oil-in-water emulsions and create foam (lather) in aqueous phases. This is their main mission (in carbonated beverages). They are virtually non-toxic by ingestion, but it may be kept in mind that they are extremely toxic by injection. The saponins cause haemolysis (solution of the red blood corpuscles) which can eventually cause death. Saponins are nerve-toxic to fish and many other cold-blooded creatures, and may cause paralysis by ingestion by fish ("fish-poison").

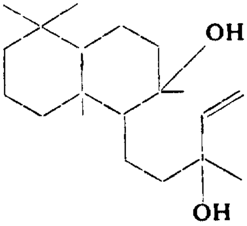
Normal concentrations of saponins have no odor and very little taste. Higher concentrations have a bitter-acrid taste, and some saponins are used to create this bitter-tart taste and mouthfeel. Still higher concentrations are irritating to the human mucous membranes.

G.R.A.S. by F.E.M.A.

100-920; 124-129; 162-711;

## 2836: SCLAREOL

A di-*tertiary*, bicyclic Glycol.



$C_{20}H_{36}O_2 = 308.51$

White crystals. M.P. 106° C. Sp.Gr. (liquid) 0.96. B.P. higher than 340° C.

Insoluble in water, soluble in alcohol and oils. The solubility in alcohol is rather low, but sufficient for practical perfume compounding. The material is easily soluble in hot alcohol.

Practically odorless. Slightly bitter taste in concentrations of about 100 ppm.

Although this chemical has been known, and its existence in Nature confirmed many decades ago, it is still an object under intense research. Its olfactory relationship to Ambregris was suspected by the perfumer long before the chemist could prove the chemical relationship. Sclareol has so far been identified in only one natural product in significant amount, and that product (Clary Sage) has long been known for its outstanding tenacity and delicate Ambregris terminal notes.

Sclareol as such is rarely used in perfumery, but a great number of related, odorous chemicals with similar fixative effect are used in modern perfumes. A specially prepared Clary Sage absolute is used in tobacco flavoring in the shape of a paste, separately added, not blended with the usual flavor solution.

Sclareol is also related to key odorous components of Labdanum, again confirming what the perfumer has found many generations ago, that Labdanum products have an Ambre-effect in perfumery. Such findings and confirmations should further encourage a close co-operation between the perfumer with deep knowledge of raw materials and the research chemist with imagination and flair for modern synthesis.

The fact that Sclareol has an olfactory effect may partly be explained by the observations that oxidation products of Ambrein have odor, and they are volatile to such a degree that we can smell them (and appreciate them). The same could be true of Sclareol-derivatives.

While Sclareol is indeed commercially available, the perfumers are generally using Clary Sage absolute for the desirable perfumery effect of Sclareol plus the almost universally applicable odor of the plant extract itself. Contrary to what many perfumers may think, Clary Sage absolute is less expensive than the essential oil of Clary Sage. The latter is furthermore a very poor source of Sclareol, which is almost non-distillable with steam, and therefore very poorly represented in the essential oil.

Manool (see monograph) whose formula is "Sclareol minus $H_2O$", came into the Ambregris picture much later, but its relationship is quite obvious. It was only after that discovery, that the new, synthetic Ambregris materials were made commercially available.

Literature is abundant on the subject of Ambrein, Sclareol, etc., and the reader interested in that subject should consult expert literature. This work includes a number of chemicals related to Sclareol, and used in perfumery:

1) Abitol (2).
2) Ambrein (104).
3) Ethyldodecahydro trimethylnaphtofuran (1213).
4) Fixateur 404 (1391).
5) Manool (1835).
6) Squalene (2862).

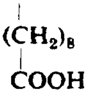
Reference is also made to the monograph on Dihydro-*gamma*-ionone (950).

Prod.: by isolation from Clary Sage absolute, which contains from 38 to 45% of Sclareol.

7-133; 67-714; 88-363; 88-365; 163-70; 163-237; 163-375; 163-172;

## 2837: SEBACIC ACID

Decanedioic acid.
Octane-*1:8*-dicarboxylic acid.



$$\begin{array}{c} COOH \\ | \\ (CH_2)_8 \\ | \\ COOH \end{array}$$

$C_{10}H_{18}O_4 = 202.25$

Prismatic crystals or leaflets, colorless crystals or white powder.

M.P. 135° C. B.P. 364° C. (sublimes at melting point). Sp.Gr. 1.21 (liquid).

0.1% soluble in cold water, 2% soluble in boiling water, soluble in alcohol and most oils, but poorly soluble in terpenes.

Mild, bland, slightly fatty odor of excellent tenacity.

The title material is briefly mentioned in this work, although it is not classified as a perfume or flavor chemical as such.

Many of its esters are used as diluents in perfumery or as "plasticizers" for Resinoids, etc., while salts and other derivatives of the acid are extensively used in cosmetic preparations.

It is therefore of some importance to know the odor type of this acid, since it may appear in traces in the solvents, and in larger amounts in the cosmetic base materials.

Strontium sebacate is used as a powder base in cosmetics.

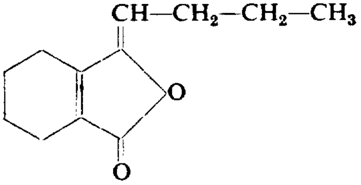
Prod.:

1) by dry distillation of Castor oil with Sodium hydroxide.
2) by ozonization of Undecylenic acid (the acid is also obtained from Castor oil).

26-676; 66-986; 100-926; 155-360; B-II-718;

## 2838: SEDANOIC ANHYDRIDE

Sedanoic acid, anhydride.
The enol-lactone of Sedanoic acid.
$\Delta_2$-Tetrahydro-*n*-butylidene phthalide.



$C_{12}H_{16}O_2 = 192.26$

Colorless, oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and warm, spicy-condiment-like, sweet odor of good tenacity.

The flavor at concentrations lower than 5 ppm is Celery-Lovage-like, warm, spicy, but not pungent or burning.

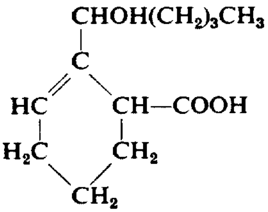
The title material has been suggested as a modifier for flavor compositions aiming at imitation Celery and Lovage flavors, particularly for soaps.

Although this material may not be a natural component of Celery and Lovage, it is very closely related to the key flavor principles of those natural materials. Its character is somewhat sharper than the type of Dihydrobutylidene phthalides, and less deep-warm, but the material performs well in combination with the homologues.

67-234; 90-625;
see also: Journal of Food Science, vol. 28, page 640ff.

## 2839: SEDANOLIC ACID

2-(*alpha*-Hydroxyamyl) cyclohex-2-ene-1-carboxylic acid.
2-(Pentylol-2')-cyclohexen-2-carboxylic acid-1.



$C_{12}H_{20}O_3 = 212.29$

White, needlike crystals. M.P. 89° C. Very slightly soluble in water, soluble in alcohol, somewhat soluble in oils, but not all.

Upon heating or drying out under improper storage, the acid will lose water and form Sedanolide (see that monograph).

The anhydride has a much stronger odor than the acid, and older samples of the acid may therefore smell stronger.

This acid, although naturally occurring in Celery seed oil and extract, is of very little interest as such. It contributes only a minor part of the flavor of Celery, and plays more of a chemical role in stabilizing and establishing an equilibrium of acid/lactone in the natural product. The lactone is destroyed by action of alkali and the acid offers a temporary protection against such process in the natural material.

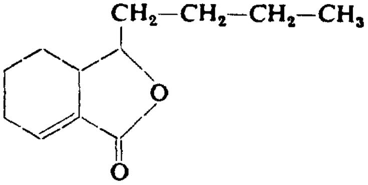
However, with proper composition of artificial Celery flavor, and proper selection of diluents and blenders, it is generally not necessary to use the acid at all in flavor compositions.

The lactone can be prepared synthetically by methods completely avoiding the acid. Accordingly, the acid is not a common commercial product.

67-231; 90-177; 105-909; 96-176;

## 2840: SEDANOLIDE

Sedanolic acid, lactone.
$\Delta_3$-Tetrahydro-*n*-butylphthalide.
*2*-(*alpha*-Hydroxyamyl)-cyclohex-*2*-ene-*1*-carboxylic acid, lactone.



$C_{12}H_{18}O_2 = 194.28$

Colorless or pale straw-colored, slightly viscous liquid. Sp.Gr. 1.04. B.P. 284° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm, herbaceous-spicy and very tenacious odor, suggestive of Celery.

Warm and spicy, in extreme dilution Celery-like taste with no pungency at concentrations below 5 ppm.

The title material was once considered the key flavor principle of Celery. This statement has been seriously questioned, and many homologues and related materials have later been identified and named key flavor components of Celery. It appears that the title material (under that structure) may not be present in Celery seed at all, while several very closely related phthalides are so.

The fact remains that the title material has a pronounced Celery-like odor, and so has many other materials, not identified in Celery or elsewhere in Nature (yet).

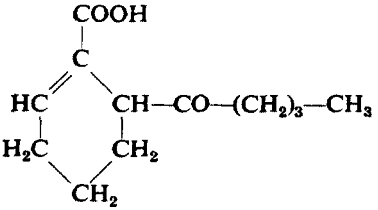
This lactone is used in flavor compositions aiming at reconstituting Celery flavor, particularly for processed food, soups, condiments, dressings, etc.

It should be noted, however, that *none* of these lactones, anhydrides and related materials, including those identified with certainty in Celery, are included in the American G.R.A.S. list.

67-231; 90-623; 95-191; 96-176; 104-150; 158-145; 159-675; 65-694;
See also monographs:
Dimethyl hydroxybutyl butenolide (1024).
Methyl propyl cyclohexenone (2215).

## 2841: SEDANONIC ACID

*2*-(Pentylon-*2'*)-cyclohexen-*6*-carboxylic acid-*1*.
*6*-Valeryl cyclohex-*1*-ene-*1*-carboxylic acid.



$C_{12}H_{18}O_3 = 210.28$

White or colorless crystals. M.P. 113° C.

Very slightly soluble in water, slightly soluble in oils, soluble in alcohol.

Faint, but tenacious warm-woody, spicy and slightly camphoraceous odor.

This ketoacid, occurring in Celery seed Oleoresin, has been suggested for use in flavor compositions, particularly spice blends, imitation Celery or artificial or "reinforced" Celery seed extract, but is very rarely offered commercially.

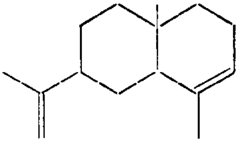
The lactone, corresponding to the hydrogenated ketoacid (see Sedanolide) is generally considered of more interest, and so are several related derivatives, all of which are produced synthetically by methods bypassing the subject ketoacid.

Most conceivably, this material will remain on the research shelf and be of purely academic interest in the future.

90-183; 67-234; 105-909;

## 2842: alpha-**SELINENE**

*1,10*-Dimethyl-*7*-*iso*-propenyl-octahydronaphthalene.
Formerly known as *alpha*-Eudesmene.



$C_{15}H_{24} = 204.36$

Colorless or pale straw-colored, oily liquid. B.P. 258° C. Sp.Gr. 0.91.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet-woody, slightly peppery odor of good tenacity.

This sesquiterpene has a history of brief interest to perfumery. When it was identified in "Bois de Rose" oil from Brazil and Peru, it was considered of interest to the work on artificial Bois de Rose oil, particularly when the low-cost synthetic Linalool appeared on the market in the early-to-mid-1960's.

In spite of continuously lowered prices on Linalool (synthetic), the price of Bois de Rose oil has not fallen below its "medium" level, which is almost twice the cost of synthetic Linalool today. And Bois de Rose oil maintains a firm interest in certain circles of the perfumery world.

This sesquiterpene has been suggested for use in perfume compositions as a fixative in floral spicy and woody fragrance types.

However, since the hydrocarbon itself is not readily available as a major component of any common essential oil, there is little chance that the material will ever become a standard perfume material.

The above material is also interesting in connection with the temporary use of Eudesmyl acetate during World War II as a substitute for Linalyl acetate. Eudesmol can be produced from Eudesmene. Both are present in Australasian Araucaria oil, but have otherwise never become of any importance to perfumes. But there is a peculiar physiological and olfactory relationship between these materials.

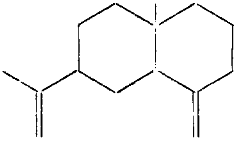
Prod.:

1) by isolation from Brazilian Bois de Rose oil.
2) by dehydration of Eudesmol (see monograph 1367).

67-642; 87-274; 95-79; 96-57; 159-622; 88-273;

## 2843: beta-**SELINENE**

*10*-Methyl-*1*-methylene-*7*-*iso*-propenyl-decahydronaphthalene.



$C_{15}H_{24} = 204.36$

Colorless or pale straw-colored oily liquid. Sp.Gr. 0.92. B.P. 269° C.

Insoluble in water, soluble in alcohol and oils.

Mild, woody, warm, herbaceous-peppery odor of excellent tenacity. Less peppery than *alpha*-Selinene, but warmer, more herbaceous.

The Selinenes are generally not available on a commercial scale.

The title sesquiterpene is briefly mentioned in this work to further elucidate the relationship to some better known perfume chemicals (referring to *alpha*-Selinene), while *beta*-Selinene is of little more than academic interest.

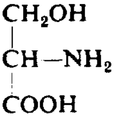
Celery seed oil has never been in such strong demand, or such poor availability or high price, that any serious attempt has been made to make an artificial or "reconstructed" Celery seed oil. The title material would be a potential component of such product, probably to the extent of about 10%.

Prod.: so far only by isolation from Celery seed oil. No useful synthesis has been developed (see above remarks).

67-642; 87-277; 95-78; 96-57;

## 2844: SERINE

*beta*-Hydroxyalanine.
*alpha*-Amino-*beta*-hydroxypropionic acid.



$$\begin{array}{l} CH_2OH \\ | \\ CH-NH_2 \\ | \\ COOH \end{array}$$

$C_3H_7NO_3 = 105.10$

Exists as hydrate and in anhydrous form.

White powder.

Decomposes when heated to 228° C.

5% soluble in cold water, 33% soluble in boiling water.

Insoluble in alcohol and oils.

Virtually odorless when pure.

Mild, sweetish taste in aqueous solutions of concentrations near 1000 ppm (0.1% and higher).

The title material is not classified as a flavor material, but it is used quite extensively as a dietary nutrient, and the fact that it has a sweet taste may be of interest to the flavorist.

Serine has been used as component of Maple imitation flavor. The title Aminoacid is not used in perfumes.

G.R.A.S. (also the hydrochloride salt).

Prod.:

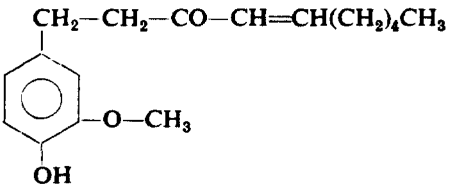
1) as a by-product in the manufacture of silk (silk-gum).
2) synthetic – from Ethyl acrylate, or by condensation of Ethyl formate with Ethyl hippurate, followed by reduction and hydrolysis.

Many other synthetic methods are known.

58-III-54; 60-V-59; 66-1068; 100-931; 162-711;

## 2845: SHOGAOL

*1*-(*4*-Hydroxy-*3*-methoxyphenyl)-*4*-decen-*3*-one.
(*4*-Hydroxy-*3*-methoxyphenyl)-ethyl-*n*-*alpha*-*beta*-heptenylketone.
A part of "Gingerol".



$C_{17}H_{24}O_3 = 276.38$

White crystalline powder. B.P. higher than 300° C.

Very slightly soluble in water, soluble in alcohol and oils.

Mild, warm-herbaceous, sweet odor.

Pungent, spicy-warm taste at concentrations higher than 5 ppm.

This ketone is one of the pungent principles in the Ginger rhizome and in the Oleoresin made from that natural material.

Shogaol has little or no application in perfumery, and very little interest to the flavor industry, but it is included in this work mainly for the purpose of elucidating the problems apparently existing around the description of the odor and flavor of "Zingerone".

The author feels, that the common description of Zingerone as being "pungent principle of Ginger" must be an unfortunate confusion of the sweet-and-warm, spicy tasting, but absolutely non-pungent ketone (Zingerone), with the title material, or its higher or lower homologues, all present in Ginger. In fact, the higher homologue is considered a major contributor to the pungency.

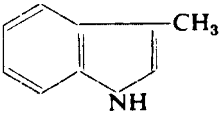
It is useful to remember that these (three) ketones lose their pungency by treatment with alkali. Potassium carbonate is often used in spice cookies to increase the crispness or brittleness. But it would also destroy all or part of the Ginger pungency if Ginger Oleoresin or Ginger powder were used in the cookie dough.

Prod.: by condensation of Vanillin with Acetone, followed by hydrogenation. The resulting ketone (Zingerone) is then condensed with Hexaldehyde under conditions which inactivate the hydroxyl group during the reaction. Valeraldehyde or Heptaldehyde instead of Hexaldehyde will yield the two other pungent principles.

1-523; 68-990; 130-204;

## 2846: SKATOLE

*beta*-Methylindole.
*3*-Methylindole.



$C_9H_9N = 131.18$

White crystals, becoming reddish or brownish upon exposure to air and daylight.
M.P. 96° C. B.P. 266° C.

Very slightly soluble in water, soluble in alcohol and oils.

Very powerful and diffusive, also extremely tenacious odor, in high concentration repulsively unpleasant, only in very low concentration pleasant, sweet, warm, animal, with a note of overripe fruit.

The fecal note generally described, and probably also observed in Skatole, may be due to trace impurities, although the material itself does exhibit an odor of decaying animal tissue, this note is more pronounced in certain grades of Skatole than in others.

The taste of Skatole is warm, overripe fruity at concentrations below 0.1 ppm, while it becomes more animal near 1 ppm.

Skatole is used in perfume compositions and in artificial Civet bases. Minute traces of this material may introduce just that natural note of "overmature flower" or "forest-floor" or other natural decomposition matter, which can be not only tolerable to a fragrance, but sometimes make it much more attractive.

The use in Civet is quite common, since Skatole is a natural component of that material. It is often used in combination with Phenylacetates and Civettone or related macrocyclic ketones.

Many perfumers have never used Skatole, and others have had poor results with it. It takes considerable patience to study the full and final effect of a certain amount of Skatole in a fragrance. The material seems to "grow" after some time of ageing, and it produces more obnoxious odors with certain materials than with others. Skatole gives interesting effects with Sandalwood materials.

The use of Skatole in flavors may come as a surprise to some perfumers who find it hard to believe that we can "eat" this odor. But minute traces are useful in Grape and Cheese imitation flavor, fruit complexes, Nut flavors, etc., highest in Cheese flavor. Concentrations in the end product vary from 0.01 to 1 ppm.

Prod.:

1) from Propionaldehyde-phenylhydrazone with Zinc chloride.
2) from Indole and Ethyl nitrite plus Sodium ethoxide via *beta-iso*-Nitrosoindole to Skatole.

3) from Acetyl-*meta*-toluidine in Diethylamine with Potassium-*tertiary*-Butoxide at high temperature.

4) an old, abandoned synthesis used Strychnine, treated with Calcium hydroxide. This has intrigued many writers of detective stories, where they will let the master detective "quick-analyze" the alleged poison with lime (Calcium hydroxide) and produce a repulsive odor (of Skatole).

5) Skatole occurs as a natural breakdown product of Tryptophan. This explains partly the occurrence of Skatole in human faeces.

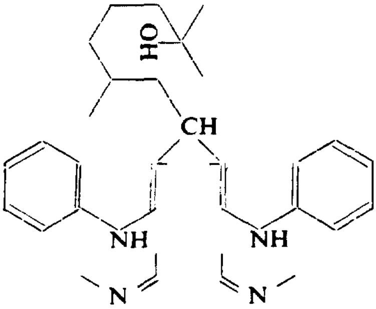
G.R.A.S. F.E.M.A. No.3019.

1-789; 1-791; 68-84; 95-205; 96-222; 106-329; 156-192; 163-376; 163-237; 163-70;

## 2847: SKATOLENE

Skatole-hydroxycitronellal ("Schiff's base"). *2,6*-Dimethyl-*8,8bis*-(*3*-methyl-*3H*-indol-*3*-yl)-*2*-octanol.

(The structure below is one of two structures usually suggested for the material).



alternative:

$C_{28}H_{36}N_2O = 416.61$

Pale straw-colored, very viscous, at room temperature non-pourable liquid.

Very slightly soluble in water, soluble in alcohol and oils.

It is customary to keep the material is suitable dilution, so that it is pourable. This prevents harmful, intermittent heating, which would discolor the material and further increase the viscosity.

A 50% solution in Diethylphthalate is viscous, but pourable at room temperature.

According to the origin of the material, Skatolene shows great variation in odor. The type of Skatolene showing an intensely warm-animal odor, tenacious, sweet and uniform, with no traces of fecal note, is generally a preferred one. Skatolene is used for floral complexes, where animal notes are tolerable or desirable. It should add warmth, depth, tenacity and life to such fragrance types, and Skatolene can be used quite freely, in amounts often surprising the perfumer unless he is very familiar with the effect of Skatolene.

Concentrations up to several percent of this material can be experienced without any offensive effect. In Gardenia, Narcisse, certain types of Rose, and in heavy exotic or Oriental fragrance types, the title material can add very attractive character.

Prod.: by condensation of Skatole with Hydroxycitronellal in the molecular proportion of 2:1.

Other condensation products of Skatole with Aldehydes are known.

See also monograph: Indolene.

## 2848: SODIUM ACETATE

$CH_3COO-Na + H_2O$

$C_2H_3NaO_2 = 82.04$

$C_2H_3NaO_2, 3H_2O = 136.09$

Colorless crystals or white granules.

The material melts in its own water at 58° C. and becomes anhydrous at 120° C.

Solubility: 55% in water, 16% in alcohol. Poorly soluble in oils.

Aqueous solutions have alkaline reaction.

Odorless, but may have a faint acidulous odor in moist air.

Bland saline-soapy taste, unless concentration is lower than 500 ppm. No perceptible taste below 200 ppm.

The title material is classified as a food additive, not as a flavor material. It has been included in this work among an (incomplete) number of chemicals, used in the preparation of food, and of some importance to the flavor of the product.

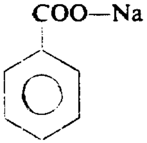
Smaller amounts up to 200 ppm are used in cereals, candy, baked goods, etc. It will also assist in maintaining crispness in cereals and baked goods. In candy it is usually an acidity/alkalinity buffer.

G.R.A.S. F.E.M.A. No.3024.

Prod.: from acetic acid.

100-942;

## 2849: SODIUM BENZOATE



$C_7H_5NaO_2 = 144.11$

White granules or crystalline powder.

35% soluble in water, 1.5% soluble in alcohol, poorly soluble or insoluble in perfume and flavor oils.

Odorless.

Sweet taste, but in concentrations higher than 1000 ppm it has an astringent taste or mouthfeel.

Sodium benzoate is used as a preservative and it has no mission as a flavor material or perfume ingredient.

To be effective as a fungistat or preservative, the material must be incorpororated in acid or mildly acid media. It is of little or no effect in alkaline solution.

Concentrations in finished products vary from 12 ppm in chewing gum and 40 ppm in Ice cream up to 1000 opm (which is maximum permissible in the U.S.A.) in fruit preserves, pickles, etc. Normal concentrations in these products are near 350 ppm, and the material is often used in combination with other fungistats.

Sodium benzoate is also used in Oleomargarine, where fungoid action would cause destruction of the flavor.

Prod.: from Benzoic acid.

G.R.A.S. F.E.M.A. No.3025.

100-945; 162-142;

## 2850: SODIUM BICARBONATE

Sodium acid carbonate.
Sodium hydrogen carbonate.
"Natron".

$NaHCO_3 = 84.01$

White crystalline powder.

10% soluble in water, almost insoluble in alcohol. Insoluble in oils.

The material loses Carbon dioxide when heated above 50° C., and at 100° C. it becomes entirely Sodium carbonate.

Odorless. Mildly alkaline, also saline, taste at concentrations above 500 ppm.

The title material, which is commonly used as a home remedy against excess stomach acid – contrary to many claims that it should not be used for that purpose – finds wide use as a component of baking powder, additive to effervescent salts, carbonated beverages, etc. and as a food additive in general.

Prod.: from Sodium carbonate with Carbon dioxide and water.

G.R.A.S.

100-946;

## 2851: SODIUM CHLORIDE

Salt.

$NaCl = 58.45$

Colorless or white, transparent or opaque crystals or granules.

26% soluble in water, 8% soluble in Glycerin, poorly soluble in alcohol, insoluble in most oils.

Odorless. Clean, saline taste, pleasant at 10000 ppm, barely perceptible at 2500 ppm. The Oceans have a salt content varying from less than 3% to more than 4%. That level is generally considered "higher than pleasant" level of salt concentration. However, the traces of other salts, including Magnesium salts, add to the bitterness and unpleasant taste of Ocean water. The optical fluid (in the human eye) is about 9000 ppm of salt, and we find our tears salty, but not unpleasantly salty.

Salt is widely used as a food additive and preservative, also as a synergist with other preservatives (Sodium benzoate, etc.).

Sodium chloride represents the typical taste "salt" of our four basic tastes: salt, sour, sweet, bitter.

Prod.:

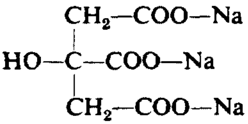
1) by mining ("rock" salt).
2) by evaporation of subterranean, salty waters.
3) by solar evaporation of sea water ("Ocean salt").

G.R.A.S. F.D.A.

100-948; 159-267;

## 2852: SODIUM CITRATE

Trisodium citrate.
"Citratin".
"Citrosidine".



$$\begin{array}{l} \qquad CH_2\text{—}COO\text{—}Na \\ HO\text{—}C\text{—}COO\text{—}Na \\ \qquad CH_2\text{—}COO\text{—}Na \end{array}$$

Penta-Hydrate: $C_6H_5Na_3O_7 + 5H_2O = 348.16$
Di-Hydrate: $C_6H_5Na_3O_7 + 2H_2O = 294.11$
Anhydrous: $C_6H_5Na_3O_7 = 258.08$

White crystals or granules. The Penta-hydrate loses water upon storage unless very well closed from air.

42% soluble in water, 60% in boiling water. Insoluble in alcohol and oils.

Odorless. Slightly salty, but pleasantly cooling taste in concentrations near 5000 ppm. The cooling effect is not perceptible much below that level. This effect resembles the effect of Potassium or Sodium Nitrates, but the Citrate is not quite as cooling.

This material is used as a sequestering agent and as a food additive. Up to 1000 ppm is used in evaporated milk, and up to 4000 ppm in toppings or icings, while the concentration in other finished products will vary from 15 to 600 ppm.

A concentration of 2000 ppm prevents blood coagulation (clotting) in the preparation of meats.

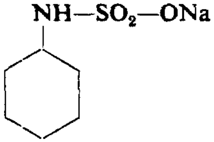
Prod.: from Citric acid.

G.R.A.S. F.E.M.A. No.3026.

100-949;

## 2853: SODIUM CYCLAMATE

Sodium cyclohexane sulfamate.
Sucaryl sodium.
Assugrin.



$C_6H_{12}NNaO_3S = 201.23$

White crystals or crystalline powder.

16% soluble in water, 4% in Propylene glycol, practically insoluble in alcohol and oils.

Odorless. Sweet taste, perceptible at concentrations higher than 100 ppm in water. The sweetening power of the title material is approximately 30 times that of sugar (sucrose) at normal use level. The fact that the minimum perceptible is almost 70 times lower than that of sugar is not completely reflected in the actual sweetening effect at concentrations near 800 ppm, where it is approximately equivalent to 25000 ppm of sugar.

Sodium cyclamate is therefore often used in combination with sugar or with Saccharin (sodium) for a more pleasant and complete sweetening effect.

As an example, the title material is permitted for sweetening of ham at the rate of 300 ppm.

See also monograph: Saccharin, for comments about the general use of non-nutritive sweeteners, and the combination-use with sugar or with other sweeteners.

G.R.A.S.

Prod.: see Cyclohexane sulfamic acid (Cyclamic acid).

See also monograph: Calcium cyclamate.

100-310; 162-503;

NOTE: Magnesium cyclamate and Potassium cyclamate are also used for above mentioned purposes, and they are listed as G.R.A.S. (by F.D.A.) as non-nutritive sweeteners.
162-657; 162-699;

## 2854: SODIUM HEXAMETAPHOSPHATE

Sodium metaphosphates.
"Calgon".
"Giltex".
"Quadrofos".
"Micromet".
"Hagan Phosphate".

mainly: $(NaPO_3)_6$

White powder or flakes. Soluble in water, slightly soluble in Glycerin, insoluble in alcohol and oils.

Although this material was developed and is marketed mainly as a water softener and detergent, it has found some use as a sequestrant in food products, for which use it has been approved in the U.S.A.

Traces of metals in food may serve as catalysts in the undesirable process of oxidation, which inevitably leads to a change in flavor, a loss in flavor or other unwanted changes.

Sequestrants are used to "hold" such metal traces and inactivate them, thus preventing or delaying the oxidation processes.

Sequestrants are therefore generally used in combination with Antioxidants, although the effect of the sequestrant is not synergistic in the original meaning of the word, they work together and produce an improved, increased effect of protection.

The title material may be used at the rate of 500 to 7000 ppm in Cereals, Wine and Gelatins, highest in the latter.

Sodium hexametaphosphate is only one out of many sequestering agents generally permitted as food additive. Some of the better known sequestering agents are:

Ethylene diamine tetra-acetate (Sodium-Calcium salt or acid Sodium salt). This material is known as E.D.T.A.

Tartaric acid and Sodium tartrate.

Sodium thiosulfate.

Calcium- or Sodium gluconate.

Citric acid and many salts and esters of same.

Phosphoric acid and many salts of same.

etc.

G.R.A.S. F.E.M.A. No.3027.

100-953;

## 2855: SODIUM HYDROXIDE

Caustic soda.
Sodium hydrate.

NaOH = 40.01

Fused solid material of crystalline structure. M.P. 318° C.

Commercial Sodium hydroxide comes in fused lumps, sticks, pellets, scales or in concentrated aqueous solution.

It absorbs moisture and Carbon dioxide from the air.

Practically odorless. Aqueous solutions have a typical "alkaline", bland, "soapy" taste at concentrations below 500 ppm (it is not adviseable to taste the material stronger).

Many chemists and some perfumers have undoubtedly made the observation that a concentrated aqueous solution of Sodium hydroxide has an odor, or, more correctly, it gives a sensation of "tasting soap" or smelling very dry dust, etc., etc. It is beyond doubt, that there is a very strong olfactory (or organoleptical) sensation. Scientific books have given no explanation on this, but the author wishes to express some theories for further thought:

1) NaOH-molecules actually do leave the solution and travel through the air to the nostrils and our receptacles?
2) The air above a saturated aqueous NaOH-solution is chemically affected by the strong affinity of the NaOH to the moisture and $CO_2$ in the air, thereby changing the composition of the air above the alkaline solution – and produce an odor sensation?

Sodium hydroxide is strongly corrosive to animal tissue. An aqueous solution at 0.5 % NaOH has a $p_H$ of 13, which is harmful to the skin.

However, the use of Sodium hydroxide in flavors is generally confined to that of being an auxiliary chemical in the process of making Caramel, treating starches, adjusting acidity, etc. in food products.

It is classified as G.R.A.S. by the American F.D.A. (food additive).

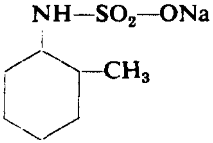
Prod.:

1) by electrolysis of Sodium chloride solution.
2) from Calcium hydroxide and Sodium carbonate (Soda).

100-953; 162-716; (Dow Chem. Co. data).

## 2856: SODIUM-ortho-METHYLCYCLOHEXYL SULFAMATE

"Homo-sodiumcyclamate".



$C_7H_{14}NNaSO_3$ = 215.30

White crystalline powder.

Soluble in water, slightly soluble in alcohol, almost insoluble in oils.

Practically odorless.

Sweet taste at dilutions of not less than 40 ppm in water.

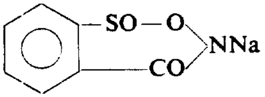
The sweetening power equals approximately 100 to 150 times that of cane sugar.

This chemical, closely related to a very commonly used sweetener, is being used as a sweeteneing agent in dietetic food and low-calorie or non-nutritive food, usually in combination with Saccharin or other sweeteners.

161-328;
see also monograph: Sodium cyclamate.

## 2857: SODIUM SACCHARIN

Saccharin, Sodium salt.
Soluble saccharin.
Sodium-*ortho*-benzosulfimide.
"Crystallose" (original name of Heyden, A.G.).



(crystallizes with 2 Mol. water)

$$C_7H_4NNaO_3S + 2H_2O = 241.21$$

White crystals, granules or crystalline powder. (Anhydrous is powder). Freshly manufactured, granular crystals are usually colorless.

The hydrate contains approximately 15% water and 85% anhydrous salt. Sweetening power of anhydrous salt: approximately 350 times that of sugar. 30% soluble in water, 2% soluble in alcohol, practically insoluble in oils.

The aqueous solutions are almost neutral.

Odorless. Intensely sweet taste, perceptible at concentrations of 15 to 20 ppm, sometimes lower. Concentrations of 100 to 200 ppm are very sweet, but relatively pleasant, and they leave only a faintly tart aftertaste, not bitter, but "unnatural" and undesirable.

Sodium saccharin is therefore often used in combination with a low-power sweetener (Cyclamate type) in the ratio of 1:12 (8-10% Saccharin sodium and 92-90% Cyclamate).

However, enormous quantities of Saccharin sodium are consumed as single sweetener in Tea, Coffee and many foods, mainly for reasons of "weight" control and not only by "people who must restrict their intake of sugar" as recommended by U.S. Government regulation.

The title material is used at the rate of 10 to 2600 ppm in various finished foods, highest in "dietetic" candy, etc. It is also used in toothpaste, normally at the rate of 1000 to 1200 ppm, depending upon the type of flavor, and also depending upon the base (highest in Fluoridetypes).

See also comments under the monograph: Saccharin.

Prod.: see monograph: Saccharin.

G.R.A.S. F.E.M.A. No.2997.

Other Saccharins listed in this work: Ammonium saccharin and Calcium saccharin.

26-674; 100-915; 159-517; 162-508;
B-XXVII-170;

## 2858: SORBIC ACID

*2,4*-Hexadienoic acid.
*2*-Propenyl acrylic acid.
The commercial product is normally the *trans-trans*-isomer form.

$$CH_3—CH{=}CH—CH{=}CH—COOH$$

$$C_6H_8O_2 = 112.12$$

White, needle-like crystals or crystalline powder. Polymerizes easily under exposure to air. M.P. 135° C. B.P. 228° C. under decomposition.

0.2% soluble in water, 3.5% in boiling water, 5.5% in Propylene glycol, 13% in alcohol. Poorly soluble in Glycerin and oils.

Pure Sorbic acid is practically odorless, but commercial grade material may have a slight, peculiar odor, varying according to the method of synthesis used.

Mild, acidulous taste in aqueous solution.

This acid is widely used as a fungistat (antimycotic) in food products and beverages, candy, etc. Its Calcium salt is commonly used for impregnating wrappers and cartons containing food which may easily spoil by oxidation (Cereals, Potato chips, etc.).

The acid is the only preservative permitted in the U.S.A. for treatment of natural cheese. It is extensively used in Pickles, Baked goods, Powder cake-mixes, Oleomargarine, Bread, soft drinks, etc.

For efficiency of this acid, the pH of the food product must be on "the acid side" i. e. not higher than 6, at which level it will prevent or delay further growth of mold and yeast, but not bacteriae.

Sorbic acid will not "kill" or eliminate existing mold and yeast, and it may, in certain cases, become metabolized by the microorganisms, particularly if the food product is seriously contaminated.

The Potassium salt of this acid is very easily soluble in water, and it may be preferred in cases of solubility problems. With suitable acidity (see above) the Potassium salt acts antimycotic as the acid, and contributes very little, if any, taste at all to the food.

Prod.:

1) by polymerization of Acetaldehyde. The trimer is Sorbic aldehyde, which can be oxidized to the acid.
2) from Malonic acid and Crotonaldehyde in Pyridine solution.
3) from Ketene plus Crotonaldehyde with Boron trifluoride.

Sorbic acid was first isolated from the juice of the unripe berries (fruits) of the Mountain Ash (Sorbus aucuparia) in which it exists as Parasorbic acid, a lactone, together with Malic acid.

G.R.A.S.

66-645; 100-968; 162-250; B-II-483; 140-145;

## 2859: SORBITAN MONOSTEARATE

"Span 60" (Atlas Powder Co.).
A partial ester of Stearic acid with Hexitol anhydrides (Sorbitans).

The title material is briefly mentioned in this work as an example of oil-soluble emulsifiers, permitted and used in food products.

The water-soluble emulsifiers are mentioned under the title Polysorbate, see that monograph.

Concentrations of 10 to 8000 ppm are used in various finished food products, highest in candy and baked products, while the concentration in certain types of icings and coatings may be even higher (up to 10000 ppm).

Sorbitan monostearate is a viscous, pale yellowish or straw-colored liquid, soluble in oil and fats.

It has only a very faint, oily-waxy odor, and a bitter taste in concentrations higher than 1000 ppm. However, its insolubility in water, and the fact that it is used mostly with large amounts of sugar (and acid) account for the much higher use level without any serious influence upon the flavor of the finished product.

Concentrations of 1% (10000 ppm) of the title material in plain water with or without 5-8% sugar, are rather unpalatable.

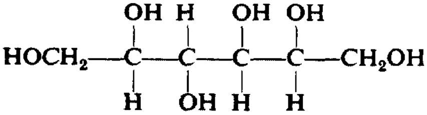
G.R.A.S. F.E.M.A. No.3028.

The U.S. Federal Register gives very detailed description and limitation for the use of the title material and related emulsifiers. They are also permitted for use as de-foaming agents.

100-970;

## 2860: SORBITOL

*dextro*-Sorbitol.
*dextro*-Glucitol.
*dextro*-Sorbite.
*dextro*-Sorbol.
*1,2,3,4,5,6*-Hexane-hexol.
"Sorbo".
"Karion".
"Sionon", and numerous other trade names.



$$HOCH_2-\underset{H}{\overset{OH}{C}}-\underset{OH}{\overset{H}{C}}-\underset{H}{\overset{OH}{C}}-\underset{H}{\overset{OH}{C}}-CH_2OH$$

$C_6H_{14}O_6 = 182.18$
$+ \frac{1}{2}H_2O$ or $+ H_2O$.

Colorless needle-like crystals or white powder (anhydrous). M.P. 112° C. (anhydrous).

83% soluble in water (a 70% syrup is commercially available), very poorly soluble in cold alcohol, soluble in hot alcohol, practically insoluble in oils (flavor materials).

Odorless. Pleasant, sweet taste, with a sweetening power estimated at about 60% of the power of sugar (sucrose). Sorbitol gives almost the same calorie yield as sugar, but it is metabolized by the human digestive system without appearing as Glucose in the blood, and is therefore tolerated by diabetes patients.

The commercial Sorbitol liquid (syrup) may contain some Mannitol, etc.

Sorbitol is extensively used as a moisture conditioner and a sweetener in foods. Enormous amounts are used by the tobacco industry, while thousands of tons enter food and beverages at the rate of 1000 to 280000 ppm (up to 28% in certain toppings).

It is miscible with Glycerin and Propylene glycol, and therefore appreciated in Liqueurs as a viscosity increaser, in chewing gum for "sugar-free" chewing gum, in hard candy, chocolate, Ice creams, Sherberts, etc. It is also used as a conditioner/humectant in toothpaste.

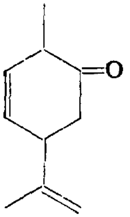
Prod.: from Glucose by electrolytic reduction or by catalytic hydrogenation.

G.R.A.S. F.E.M.A. No.3029.

100-968; 162-456;

## **2861:** laevo-**SPICATONE**

*para*-Menthadien-*5,8*(*9*)-one(*2*).



$C_{10}H_{14}O = 150.22$

Colorless mobile liquid.

Insoluble in water, soluble in alcohol and oils.

Clean, sweet, powerfully herbaceous-green, refreshing odor of Spearmint type.

Clean, sweet and very natural Spearmint-type taste, sweeter and less pungent-burning than Carvone.

This ketone has only recently been developed, and has been suggested for use in imitation Spearmint oil and flavor.

The author has no record that this ketone has been identified in Nature, and it has not yet been approved by the American authorities for use in food flavor (Nov. 1968).

The title material is an isomer of *laevo*-Carvone, and it was indeed brought on the market by one of the manufacturers interested in artificial Spearmint oil (Glidden Co., 1958, Amer. Pat. No. 2918495).

The subject ketone has not been regularly available, and it is possible that manufacturing problems, or the fact that the ketone has not been approved as G.R.A.S., are responsible for the irregular availibility of this interesting material. The synthesis starting from *laevo*-Carvone places immediately a rather high cost on the ketone, and it may not be able to compete with the large-volume-produced *laevo*-Carvone as a common Spearmint flavor chemical.

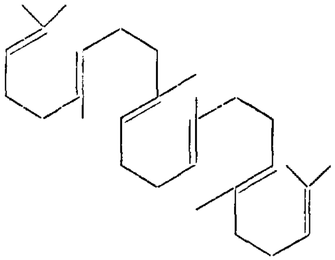
Prod.: from *laevo*-Carvone by heating with weak acid or alkali.

Sample: The Glidden Co., Jacksonville, Florida, U.S.A.

89-261;

## 2862: SQUALENE

*2,6,10,15,19,23*-Hexamethyl-*2,6,10,14,18,22*-tetracosahexaene.



$C_{30}H_{50} = 410.73$

Almost colorless oily liquid. B.P. higher than 350° C. Sp.Gr. 0.86.

Insoluble in water, poorly soluble in alcohol. Soluble in most oils.

The material absorbs oxygen from the air and becomes more viscous, like a "drying oil".

Mild, pleasant, soft-oily odor, normally without any trace of rancid note. Excellent tenacity.

This unsaturated hydrocarbon, to a chemist a combination of six Isoprene-chains, is briefly mentioned in the present work because of its close relationship to many very important Ambregris materials.

Squalene as such is not used in perfumes, except in occasional applications as a fixative. The completely hydrogenated hydrocarbon, Squalane, is used as a cosmetic skin lubricant. It is completely stable and offers therefore an advantage over the title material.

Prod.:

1) from Farnesol via Farnesyl bromide, and with Magnesium to the title hydrocarbon. (P. Karrer, original synthesis).
2) by isolation from the unsaponifiable portion of the liver oil from certain sharks and other fish. It is the main component of the unsaponifiable fraction of shark liver oil. The material appears thus as a by-product in the isolation of natural Vitamin A.
3) Squalene is present in smaller amounts in yeast and in the human skin tallow, but only methods No. 1 and 2 have practical importance.

See monograph: Sclareol (2836) for relation to Ambregris materials.

1-60; 66-273; 100-974; 155-260; 87-400;

## 2863: STEARIC ACID

Octadecanoic acid.
Heptadecane-*1*-carboxylic acid.
The commercial product may contain substantial amounts of Palmitic acid.

$CH_3(CH_2)_{16}COOH$

$C_{18}H_{36}O_2 = 284.49$

White leafy crystals. M.P. 70° C.
B.P. 363° C. Sp.Gr. 0.85 (liquid).

Very slightly soluble in water, 2% soluble in cold alcohol, better in hot alcohol. Soluble in most oils.

Pure material is virtually odorless and has very little taste, but slightly waxy mouthfeel at concentrations higher than 1000 ppm. Ordinary or lower grades may have a faint oily-fatty odor and taste, mostly carried over from the starting material in making the acid.

Stearic acid is occasionally used in perfume compositions, mainly as a blender and waxy diluent in artifical flower absolutes or certain fragrances or bases, e. g. Mimosa, Tuberose, etc. It has practically no odor value.

The acid is used more commonly in flavor compositions and in foods. For imitation Butter and Vanilla, occasionally in Coconut, etc. the acid is used at concentrations varying from 2-10 ppm in most products up to 4000 ppm in certain types of candy (imitation chocolate, hardened chocolate coverings, etc.).

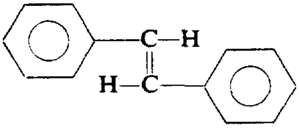
Prod.:
1) by hydrogenation of oleic acid or Cottonseed oil. This produces generally a higher grade of Stearic acid, practically free from Palmitic acid.
2) by saponification and acidification of various types of tallow. This yields poorer grades of Stearic acid with substantial amounts of Palmitic acid, etc.

G.R.A.S. F.E.M.A. No.3035.

65-564; 66-578; 90-110; 100-976; B-II-377;

## 2864: STILBENE

Toluylene.
*trans-alpha-beta*-Diphenylethylene.
This monograph includes mention of *cis*-Stilbene, formerly called *iso*-Stilbene.



$C_{14}H_{12} = 180.25$

Almost colorless or pale yellowish crystals. M.P. 124° C. B.P. 307° C.

Insoluble in water, 1% soluble in alcohol, soluble in most oils. Sp.Gr. 0.97 (liquid).

Sweet and pleasant, balsamic-floral, rather heavy odor of excellent tenacity.

This hydrocarbon is briefly mentioned because it has at one time been used in perfume compositions, and it is probably one of the oldest aromatic (Benzene-derived) perfume chemicals known (1844).

Its perfumery value today, in competition with many powerful, tenacious, inexpensive and pleasant smelling materials of similar fragrance type, is relatively poor, and one may assume that the title material is practically obsolete in modern perfumery.

It was used in Hyacinth, Lilac, Appleblossom and many balsamic-floral fragrance types, partly as a fixative.

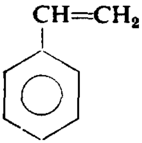
The *cis*-isomer, also called *iso*-Stilbene, is a yellowish, viscous oil of B.P. 241° C., solidifying in the cold, melting again at 6° C. This isomer is unstable and has no application in perfumery.

Prod.:
1) from Benzaldehyde plus Phenylacetic acid at 140° C. in the presence of Piperidine. This process produces *trans-alpha*-Phenylcinnamic acid as an intermediate, and the acid will be decarboxylated to the title isomer.
2) from Benzaldehyde and *2,4*-Dinitrotoluene.
3) from Benzyl magnesium chloride plus Benzaldehyde.

1-404; 31-11; 68-1142; 100-979; B-V-630; 87-413;

## 2865: STYRENE

Phenylethylene.
"Styrol".
Styrolene.
Vinylbenzene.



$C_8H_8 = 104.15$

Colorless mobile liquid. B.P. 146° C. Sp.Gr. 0.91.

Polymerizes and oxidizes easily in air, producing an odorless, glasslike resin, hard and brittle.

Poorly soluble in water, soluble in alcohol and oils.

Extremely diffusive, sweet-gassy, in dilution balsamic and almost floral odor of poor tenacity. Overall rather chemical odor, often described as prototype of "hydrocarbon" odor.

This hydrocarbon is sometimes used in minute traces in perfume compositions to enhance floral topnotes, mainly in sweet and floral fragrances for household products, detergents, etc., where radiance and diffusion of odor is often preferred over tenacity.

It is also used in certain artificial essential oils, flower absolutes, etc., not only in the reconstruction of Styrax oil and "colorless Styrax". Its floral note is suitable for Hyacinth and a few other pungent floral fragrance types.

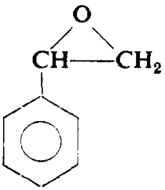
Prod.:

1) from Ethylbenzene by dehydrogenation.
2) from Ethylbenzene by chlorination, followed by dechlorination.

31-6; 87-412; 100-987; 1-403; B-V-474;

## 2866: STYRENE OXIDE

*1,2*-Epoxy-*1*-phenylethane.
Phenylethyleneoxide.



$C_8H_8O = 120.15$

Colorless liquid. Sp.Gr. 1.05. B.P. 192° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, balsamic-gassy, heavy and sweet, warm odor. Much less gassy and not nearly as diffusive as Styrene. Overall softer and very similar in odor characteristics. Fair to moderate tenacity.

This epoxide is occasionally used in the composition of artificial essential oils, e. g. Styrax oil, where the Styrene effect must be extended deeper into the fragrance, and not be quite as volatile as it will be with Styrene itself.

Apart from being a variation of Styrene with less gassy effect and better tenacity, this material has very little to offer a perfumer.

It is an important intermediate in the manufacture of various perfume chemicals, and one patent covers the catalytic hydrogenation of the title oxide to make Phenylethylalcohol. Rearrangement of the Styrene epoxide may yield Phenylacetaldehyde.

The oxide is much more stable towards polymerization and oxidation than Styrene, therefore often preferred over the hydrocarbon for the above purpose (Styrax).

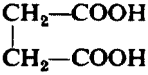
Prod.:

1) from Styrene with Perbenzoic acid.
2) from Styrene chlorohydrin with Sodium hydroxide.

68-527; 68-878; B-XVII-49;

## 2867: SUCCINIC ACID

Butane dioic acid.
"Amber acid".



$$\begin{array}{l} CH_2\text{—}COOH \\ | \\ CH_2\text{—}COOH \end{array}$$

$C_4H_6O_4 = 118.09$

Colorless or white crystals. M.P. 189° C.
B.P. 235° C. (loses water at that temperature).

7% soluble in water, 10% soluble in alcohol, 4% soluble in Glycerin. About 50% soluble in boiling water, poorly soluble in oils.

Odorless. Tart-acid, almost astringent mouthfeel and taste in aqueous solutions at concentrations higher than 2000 ppm.

This acid has found some use in flavor compositions or as a food additive, mostly to introduce the tartness, which is generally not achieved by means of conventional acids or flavor materials.

Certain berry flavors (Gooseberry, Blackcurrant, Mountain Ash, etc.) require a tartness along with the acid taste. It is also used in discrete amounts in wine flavors, etc.

Many esters of Succinic acid are used as diluents in perfumery or as mild odorants, solvents and blenders, but the acid itself has no application in perfumes.

Prod.:
1) by oxidation of Butanediol-*1,4* with Nitric acid.
2) by oxidation of Tetrahydrofuran with Nitric acid.
3) by hydrogenation of Fumaric acid or Maleic acid,
- and many other methods.

G.R.A.S.

66-968; 90-170; B-II-601;

## 2868: SUCROSE OCTA-ACETATE

Octa-acetyl sucrose.
The name "Glucose octa-acetate" is sometimes used, but it is chemically erroneous and confusing.

$(C_{12}H_{14}O_3)(OOCCH_3)_8$

$C_{28}H_{38}O_{19} = 678.61$

White powder. M.P. 84° C.

0.1% soluble in water, 9% soluble in alcohol, soluble in most oils.

Practically odorless.

Intensely bitter, but clean and not unpleasant taste at concentrations near 1 to 10 ppm. The bitter taste is strongly influenced (organoleptically, but not chemically) by the presence of food acids.

This material has no application in perfumery.

It is used as a bitter principle in many types of carbonated beverage, e. g. Ginger Ale, "Quinine"-bitters (in addition to Quinine which is expensive and scarce), various tonics, spice beverages, etc.

The normal concentration is about 10 to 20 ppm in beverages, and much lower in food products (0.2 to 0.5 ppm).

The title material is also used for the denaturing of Ethyl alcohol.

G.R.A.S. F.E.M.A. No.3038.

100-991;

## 2869: SULFUR DIOXIDE

Sulfurous oxide.
Sulfurous anhydride.

$SO_2 = 64.07$

Colorless gas. Condenses to a colorless liquid below minus 10° C.

10% soluble in water at room temperature, 23% at 0° C. 4% at 50° C. 25% soluble in alcohol.

Stinging, suffocating odor, irritating to the mucous membranes. Sharp, acid taste in aqueous solution. Minimum perceptible is about 500 ppm.

In spite of the harmful effect of the gas upon the human respiratory system, the aqueous solution is relatively harmless to the digestive system. The material is quickly oxidized to Sulfuric acid and transformed into Sulfates. The human tolerance for ingestion of the solution is therefore surprisingly high.

Sulfur dioxide is widely used as a bleaching agent and disinfectant for fruits, fruit juices, concentrated fruit juices, dried fruits, wines, beer, storage tanks, etc. It is also used for bleaching of sugar. The effect of Sulfur dioxide is strongly dependant upon the acidity of the treated material. Below an acidity of pH 2 or 3, there is a marked decrease in the effect, and at neutral the gas is practically useless.

The minimum perceptible for taste of the title material is below the level commonly used (400 to 2000 ppm) and the use of Sulfur dioxide is justified to a certain extent upon the fact that the gas will evaporate or be evaporated prior to use of the product.

Since certain metals, including iron and tin, may reduce the Sulfur dioxide to Hydrogen sulfide, the treatment with Sulfur dioxide must be restricted or avoided where the product goes into tin cans. Minute traces of Hydrogen sulfide would cause blackening of the food product and a very repulsive odor. It has been claimed that levels of Sulfur dioxide below 20 ppm are safe against such drawbacks.

Sulfur dioxide has the advantage (like Formic acid) that it can be "boiled out" of the product, provided the acidity is kept high.

For surface-treatment of fruits, including the fruits for wine-making, this is considered a major advantage.

The concentration of the title material in finished food is therefore generally limited to a few ppm up to 400 ppm (near taste level).

It is also widely used in treatment of meats and fish.

Sulfur dioxide is commercially available in pressure flasks as a liquid. It was formerly "produced" by burning of sulfur, e. g. sulfur sticks were ignited and left burning inside storage tanks, etc. for disinfection.

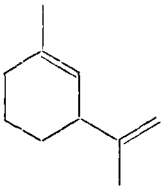
The "air pollution" of modern, large cities with heavy industry is often measured by indicating the amount of Sulfur dioxide in the air. The gas is considered approximately half as toxic as Nitrobenzene vapors, but the hazard is partly that of corrosion of the respiratory system, while the ingestion of Sulfur dioxide solution is much less harmful.

G.R.A.S. F.E.M.A. No.3039.

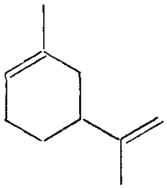
26-316; 100-1003; 100-1004; 162-164;

## 2870: SYLVESTRENE

Commercially available materials have usually been mixtures of:
*meta*-Menthadiene-*1*,*8*(*9*) and
*meta*-Menthadiene-*6*,*8*(*9*).
(*dl*-Sylvestrene is also known as: Carvestrene).
*1*-Methyl-*3*-*iso*-propenyl-*1*-cyclohexene
(or -6-).



and:



$C_{10}H_{16} = 136.24$

Colorless mobile liquid. B.P. 177° C.
Sp.Gr. 0.85.

Insoluble in water, soluble in alcohol and oils.

Refreshing citrusy, mainly lemony, odor of poor tenacity.

This Monoterpene has been suggested for use in perfume bases and artificial essential oils, since it became commercially available on a limited scale a few years ago.

However, with a restricted availability, the material has little chance of becoming truly popular for such purpose, where relatively large amounts of raw material are required.

The terpene could find use in the reconstruction of Lemon, Lime and various other large-volume essential oils.

Prod.:

1) from $\Delta_3$ or $\Delta_4$-Carene, which is obtained from East Indian Pine Needle oils, via the Dihydrochloride, followed by boiling with Aniline to obtain the title hydrocarbon.
2) from *3*-Cyclohexene-*1*-carboxylic acid.

31-7; 67-227; 67-511; 87-79; 163-376;

## 2871: TANNIC ACID

Tannin.
"Gallotannic acid".
The commercial material is a penta-di-galloyl-ester-like derivative of Glucose. There is a marked difference in the composition of the "Chinese" and the "Turkish" Tannin, but the general composition is that of one Mol. Glucose with five to ten Mols. of acid.

$C_{76}H_{52}O_{46}$ = 1701.25
(usually with 10 Mol. $H_2O$)

Pale greyish or off-white or pale brownish, fluffy, amorphous powder.

Darkens when exposed to air and daylight. Soluble 25% in water, also soluble in alcohol and Glycerin, but insoluble in most oils. The material precipitates proteins (Gelatin, Albumin, etc.) and produces condensation products with Diacetyl, many aldehydes, etc.

The aqueous solution is actually a solution of Gallic acid.

Very strictly purified material is practically odorless, while commercial grade material has a faint, peculiar woody-medicinal odor.

The taste is bitter and it gives an astringent mouthfeel.

Tannic acid is used as a bitter principle and astringent additive in many flavors, but is not always incorporated in the flavor composition. Concentrations vary considerably in the functional products, from 1 to 1000 ppm, highest in alcoholic beverages, lower in imitation Butter, Caramel, Maple, Nut, fruit complexes, etc.

The minimum perceptible of bitter taste varies according to the amount of food acid present, yet it has also been suggested that Tannic acid be added to Apple cider prior to fermentation in order to improve the flavor of the sparkling cider. Wine, which is known for its relatively high content of acid, is often rich in Tannic acid, and the storage of certain types of Brandy (including Whisky) in Oak wood tanks will inevitably introduce traces of Tannin into the alcoholic beverage. In brief, Tannin is almost always accompanied by acid in food products.

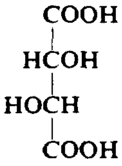
G.R.A.S. F.E.M.A. No.3042.
Prod.:
1) by extraction from Nutgalls (Chinese or Turkish), from Myrobalans (Terminalia sp.), Oakbark, etc.
2) by esterification of Glucose with *meta*-Galloylgallic acid.

It should be noted that the American authorities specify Tannic acid as "a natural flavor extractive" and that the G.R.A.S. designation therefore does not cover a purely synthetic product.

1-553; 100-1010; 159-659; 26-744; 68-812;

## 2872: TARTARIC ACID

*L*-Tartaric acid (a *dextro*-rotatory form with *laevo*-configuration).
Natural Tartaric acid.
*L-2,3*-Dihydroxy butanedioic acid.
*dextro-alpha-beta*-Dihydroxysuccinic acid.
Of the four known modifications, the "Natural Tartaric acid" is described in this monograph, since the other modifications are of little interest to the flavor industry (*DL*-Tartaric acid is only soluble 15% in water).



$$\begin{array}{c} \mathrm{COOH} \\ | \\ \mathrm{HCOH} \\ | \\ \mathrm{HOCH} \\ | \\ \mathrm{COOH} \end{array}$$

$C_4H_6O_6$ = 150.09

Colorless or translucent, white crystals or crystalline powder.

M.P. 170° C. (beginning decomposition).

56% soluble in water at room temperature, 27% soluble in alcohol, practically insoluble in oils.

Odorless. Refreshing, strongly acid taste, pleasant at concentrations lower than 5000 ppm – dependent upon sweeteners and other additives.

Tartaric acid is not used as such in perfumes, but it is commonly used as a sequestrant or, indirectly, as a bleaching agent for essential oils contaminated and colored by iron (Patchouli, Vetiver, Copaiba, Clove leaf oil, etc.).

It is widely used as an acid additive to foods and food flavors, beverages, candy, etc. The concentration may vary from 500 ppm in jellies up to 10000 ppm in condiments. Average concentrations are found in sour drops, marmelade, icecream, sherbet, soft drinks, etc. The natural concentration in Grapes is about 10000 ppm, but it is accompanied by an exceptionally high (17%) sugar content. The concentration of 500 ppm is only little higher than the minimum perceptible, and such levels of acidity are often used for flavor enhancing.

Although the title acid is said to have a very generally pleasing sour taste, it is particularly suitable for Lime and Lemon, for Currants and other berries, Grape and Wine flavors, etc. It is also popular because of its excellent solubility in water.

G.R.A.S. F.E.M.A. No.3044.

Prod.: As Potassium acid tartrate which appears as a precipitate after the fermentation process in Wine making.

*DL*-Tartaric acid can be produced from Fumaric or Maleic acids by oxidation, or from Glyoxal plus Hydrocyanic acid, followed by hydrolysis with hydrochloric acid.

1-323; 66-1170; 100-1012; 140-147; 162-262; B-III-481;

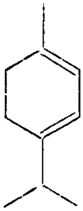
Literature on the subject of Food Chemicals is abundant in information on Tartaric acid and other food acids.

## **2873:** alpha-**TERPINENE**

*1*-Methyl-*4-iso*-propylcyclohexadiene-*1,3*.
*para*-Menthadiene-*1,3*.

The material exists in *alpha*-, *beta*- and *gamma*-forms.

The *beta*-isomer is of no interest to the perfume- or flavor industries at the present moment (Nov. 1968).



$C_{10}H_{16} = 136.24$

Colorless oily liquid. Sp.Gr. 0.84.
B.P. 176° C.

Insoluble in water, soluble in alcohol and oils.

Refreshing, lemony-citrusy odor of poor tenacity.

The taste is mostly lemony in concentrations below 40 ppm, but becomes rather bitter at higher levels.

The title terpene has recently become an article of commerce, mainly for the purpose of making it available for those interested in making artificial essential oils. It has found use in artificial Lemon oil, Mint oils, and in trace amounts in other essential oils, mainly for flavor purposes.

G.R.A.S.

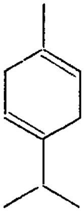
Prod.:

1) by isolation from the Terpene fraction of sweet Orange oil or "Orange terpenes". The title material may constitute as much as 8 to 10% of the total Monoterpenes.
2) by isolation from fractions of American Turpentine oil.
3) from *1*-Methyl-*4-iso*-propylcyclohexadien-*1,3*-one-*2*.
4) from Terpinene dihydrochloride with Aniline.

7-154; 67-508; 87-83; 161-456;

## 2874: gamma-TERPINENE

*1*-Methyl-*4*-*iso*-propyl-*1*,*4*-cyclohexadiene.
*para*-Menthadiene-(*1*,*4*).



$C_{10}H_{16} = 136.24$

Colorless oily liquid. Sp.Gr. 0.85.
B.P. 183° C.

Practically insoluble in water, soluble in alcohol and oils.

This isomer is the highest boiling of the Terpinenes. It has a refreshingly herbaceous-citrusy odor, not as lemony as the *alpha*-isomer, but somewhat warmer, with equally poor tenacity.

The taste is slightly bitter-herbaceous, but becomes pleasant, citrusy at concentrations below 40 ppm.

This monoterpene has found some use in the reconstruction of certain essential oils, mainly for flavor purposes: Peppermint, Spearmint, Thyme, Origanum, etc.

It is commercially available but has, to the author's knowledge, little or no application in perfumery as such. It is easily oxidized to the less desirable *para*-Cymene.

Prod.:

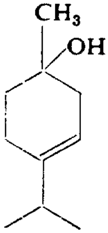
1) by isolation from the essential oil of Lantana camara, a plant growing abundantly in the West Indian islands, South America, the South Pacific islands, Indian Ocean islands, and many other tropical and subtropical areas. The plant produces an essential oil of Lavender-Clary Sage-type, but more green and harsh, yet overall very pleasant. The oil has been produced in Haiti but not on a regular basis.
2) from *para*-Cymene with Sodium and alcohol in liquid Ammonia.

G.R.A.S.

67-508; 87-90; 161-456;

## 2875: 1-TERPINENOL

$\Delta_3$-*para*-Menthen-*1*-ol.
Methyl-*4*-*iso*-propyl-*3*-cyclohexen-*1*-ol.



$C_{10}H_{18}O = 154.25$

Colorless oily liquid. B.P. 210° C.
Sp.Gr. 0.93. Solidifies in the cold.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Dry-woody, piney and somewhat musty odor of moderate tenacity.

The title material is briefly mentioned in order to complete the description of materials related to Terpineol and occurring in commercial grade Terpineol, as undesirable or desirable impurities.

This tertiary alcohol should be classified as a generally undesirable trace component of commercial Terpineol. It does not occur in all types of Terpineol, but in most of the "European type" Terpineol, manufactured from *alpha*-Pinene directly or via Terpin hydrate. The subject material would be found in the foreruns of a fractionated distillation of such Terpineol.

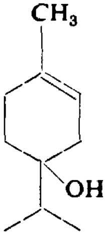
A very close relative to the title alcohol is mentioned in the next monograph, because it has achieved considerable importance in perfumery.

Prod.: from *4-iso*-Propyl-*3*-cyclohexen-*1*-one with Methyl magnesium iodide. The amounts occurring in Terpineol (see above) are insufficient for commercial production.

67-520; 88-88; 156-332;

## 2876: 4-TERPINENOL

Terpinenol.
*4*-Carvomenthenol.
*1-para*-Menthen-*4*-ol.
*1*-Methyl-*4-iso*-propyl-*1*-cyclohexen-*4*-ol.
Origanol.
The commercially available material is almost always *d*-Terpinenol-*4*.



$C_{10}H_{18}O = 154.25$

Colorless oily liquid. B.P. 212° C.
Sp.Gr. 0.92.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Warm-peppery, mildly earthy, musty-woody odor of moderate tenacity. The earthy-musty notes are pleasantly green.

The taste is rather bitter at concentrations higher than 100 ppm, while it becomes quite pleasant, warm-herbaceous, peppery below 50 ppm.

This tertiary alcohol has been known for many decades, but it was not until it had been identified in several important natural materials, that it came into the limelight of perfume chemistry and creative perfumery. It is now being used quite widely, not only in artificial Geranium, Pepper, Rose and other oils, but in many soap perfumes, perfume specialties and bases, and in flavor compositions.

One very tangible proof of its importance is demonstrated in the present cost which is about U.S. – 25.00 per kilo for a material of 85% or better purity. Not many terpene chemicals can successfully maintain such price level.

The use in flavors is mainly concentrated upon Citrus and Spice compositions, e. g. artificial Citrus and Spice oils. Concentrations may be as high as 80 ppm in Ice creams or sherbets.

Prod.:

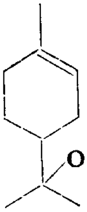
1) by isolation (fractional distillation) of Melaleuca alternifolia oil. This is the most common source today.
2) by isolation from Melaleuca linariifolia oil.
3) by isolation from Chinese or Formosan Apopin oil.
4) from Sabinene (or its isomer, *alpha*-Thujene) by hydration with dilute sulfuric acid.
5) a synthesis starting from Cineole has been suggested, but is not commercially competitive at the moment (Nov. 1968).

G.R.A.S. F.E.M.A. No.2248.

7-148; 67-519; 88-89; 104-70; 104-406; 140-127; 156-332;

## **2877:** alpha-**TERPINEOL**

*1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*8*-ol.
*para*-Menth-*1*-en-*8*-ol.
The commercial perfume grade material is mainly *alpha*-Terpineol with 3 to 5% *beta*-Terpineol and traces of other alcohols.



$C_{10}H_{18}O = 154.25$

Colorless, slightly viscous liquid.
B.P. 219° C. Solidifies in the cold, melts at 35° C. (with considerable variations according to purity). Sp.Gr. 0.94.

Very slightly soluble in water, soluble in alcohol, Propylene glycol, Mineral oil and perfume and flavor materials.

The odor of high-grade *alpha*-Terpineol being delicately floral and sweet of Lilac type, it is very strongly influenced in presence of minute amounts of impurities of different odor type. The most common undesirable odors are the more volatile terpenes and terpene alcohols (see *1*-Terpinenol) and the less volatile phenols, often occurring in traces in "European type" Terpineol. *beta*-Terpineol is the main impurity among the more volatile ones.

A "piney" odor from the more volatile impurities and a dry-medicinal odor from the less volatile ones are the most harmful olfactory notes to destroy the Lilac floralcy of perfumery grade Terpineol. It is common practise of the large users of perfumery grade *alpha*-Terpineol to purchase commercial grade Terpineol and purify their own perfumery grade from that.

Terpineol for flavor purpose should be of equally high olfactory (organoleptic) purity, except perhaps for Lime flavors, where certain qualities, unacceptable for a Lilac perfume, will be suitable for Lime flavor. But generally, a very high grade Terpineol is necessary.

*alpha*-Terpineol (or commercial Terpineol) is one of the most commonly used of all perfume chemicals. Its very low cost, excellent availability, general stability in air, soap, solvents and other chemicals, etc. and its versatility in compositions make it an everyday, all-purpose material in most perfume laboratories and compounding factories. Although exact figures are not available, the annual world consumption of Terpineol for perfumery purposes can be estimated at not less than 10,000 metric tons. However, only a relatively small portion of this volume is truly highgrade *alpha*-Terpineol, the bulk being a commercial "high-*alpha*"-grade material, which in the U.S.A. is priced very near the cost of Diethylphthalate.

As a basic component in Lilac perfumes and a major component of many varieties of Pine fragrances (lower grades of Terpineol will usually suffice) as common ingredient of Fougères, Appleblossoms, fragrances for household products, soaps, detergents, etc. it has very little competition.

Perfumers all over the world have for decades discussed the quality of Terpineol, and expressed their preference for one or the other type. It is understandable that the American perfumer is satisfied with the Terpineol most common to that continent, the Terpineol isolated from Pine oil, but it is not always easy to appreciate the terms "Lilac" for the *alpha*-Terpineol and "Hyacinth" for the *beta*-Terpineol.

The "European type" Terpineol, on the other hand, is rarely contaminated with *beta*-Terpineol (almost absent when Terpineol is made by acid hydrolysis of *alpha*-Pinene). The most annoying impurity in this type Terpineol is *iso*-Borneol, while traces of phenolic components may impair the terminal notes of that Terpineol.

It has come so far, that customers have requested *beta*-Terpineol for perfumery purposes, often and unfortunately based upon analytical information dating back prior to the use of Gas-Liquid-Chromatography as a means of analysis in combination with Infrared spectroscopy, Mass-spectometry and perhaps Nuclear Magnetic Resonance readings.

It seems beyond doubt that *alpha*-Terpineol is the most popular isomer, and the author knows of no attempt to promote a synthesis aimed at producing a higher proportion of *beta*-Terpineol in the reaction mixture than what is commonly accepted today.

The acetate of *beta*-Terpineol has been classified as "more interesting" than the acetate from *alpha*-Terpineol. This could only be welcome by the manufacturer who finds himself left with a surplus of the *beta*-isomer after vacuumdistillation of the total Terpineol.

*alpha*-Terpineol is used in discrete amounts in various flavor compositions, such as berry flavors, Lemon, Lime, Nutmeg, Orange, Ginger, Anise, Peach, etc. and in spice flavors for Frankfurter sausages, or in "Lilac" flavors. The concentration used is normally as low as 5 to 40 ppm in the finished product, highest in Citrus and Spice compositions.

G.R.A.S. F.E.M.A. No.3045.

Prod.:

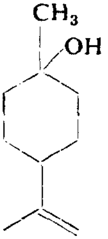
1) by isolation from American Pine oil.
2) from *alpha*-Pinene via Terpin hydrate or directly to Terpineol by hydration.
3) from Pentane tricarboxylic acid by cyclization, followed by esterification, via the Hydroxyester to the unsaturated ester, and by Grignard reagent to Terpineol.
4) from Isoprene and Methyl vinyl ketone with Methyl magnesium iodide.

Methods No. 3) and 4) are "purely synthetic" using acyclic starting materials. They are of no commercial interest as long as raw materials for methods 1) and 2) are available in volume.

34-806; 67-517; 88-55; 104-537; 104-634; 106-330; 140-127; 85-113; 156-328; 163-71; 163-238; 163-377;
Glidden Co., data sheet May 1961.
Hercules Powder Co., data sheets.
Arizona Chemical Co. data sheets.

## 2878: beta-**TERPINEOL**

*Δ-8,9-para*-Menthenol-*1*.
*1*-Methyl-*4*-*iso*-propenyl cyclohexan-*1*-ol.
The *trans-beta*-Terpineol is the most common form of *beta*-Terpineol.



$C_{10}H_{18}O = 154.25$

Colorless, slightly viscous liquid.
Sp.Gr. 0.93. Solidifies in the cold, melts again at 33° C. B.P. 210° C.

Very slightly soluble in water, soluble in alcohol and oils.

Pungent-woody-earthy, but not piney, odor of moderate tenacity.

The common odor description "Hyacinth" is a bit difficult to appreciate, particularly at first encounter with the title material.

See monograph "*alpha*-Terpineol" (preceding this) for comments on the odor of the two isomers.

*beta*-Terpineol is rarely used as such in perfume compositions, but it is a common companion to the *alpha*-isomer in commercial grade Terpineol. It has also been suggested for the manufacture of Terpinyl acetate as it is preferred by some perfumers for that purpose.

It seems beyond doubt, that the *alpha*-Terpineol is the only suitable Terpineol for better grades of Lilac fragrances and other, similar florals, while the *beta*-Terpineol is no serious drawback in Pine fragrances, Fougères and ordinary fragrances for soaps, detergents and other household products.

The author has no report of this material being used in flavor compositions.

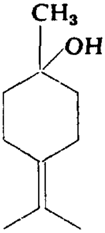
Prod.:

1) from fractions of Steam distilled Pine oil.
2) from "heads" or foreruns of the rectification of Terpineol made via *alpha*-Pinene and Terpin hydrate.
3) by reduction of Limonene epoxide.

67-517; 88-82; 106-330; 156-328; 163-71; 163-238; 163-377;

## **2879:** gamma-**TERPINEOL**

*Δ-4,8-para*-Menthenol-*1*.
*1*-Methyl-*4*-*iso*-propylidene cyclohexanol-*1*.



$C_{10}H_{18}O = 154.25$

Colorless or white prismatic crystals.
M.P. 70° C.

Very slightly soluble in water, soluble in alcohol and oils.

Soft and pleasant, sweet, almost floral odor of moderate tenacity.

The title material is included in this work mainly for the sake of completing the description of the Terpineols.

If this isomer could be manufactured separately at a cost near – or in competition with – *alpha*-Terpineol, one would have reason to believe that it could become a large-volume perfume material for everyday use.

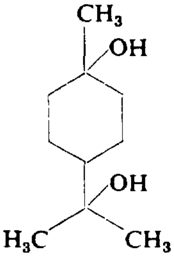
Until then, it will remain a rarity on the research shelf, and the perfumer may only smell it once in a while, when the analytical chemist calls him in for identification of some brief "whiffs" of odorous air, exhausted from the Gas-Liquid-Chromatograph vent.

Prod.:
1) by isolation from fractions of the Terpineol rectification (U.S.A.).
2) from Mesityloxide plus Acrylonitrile, followed by hydrolysis, cyclization, decarboxylation and Methyl Grignard reaction.

67-517; 88-86; 156-333; 163-238;

## **2880: TERPIN HYDRATE**

Dipentene glycol.
*trans-1,8*-Terpin hydrate.
*1*-Methyl-*4*-*iso*-propylcyclohexanediol-*1,8*, hydrate.
*para*-Menthanediol-*1,8*-, hydrate.
The Monohydrate of Terpin, a *para*-Menthane glycol.



$+ H_2O$

$C_{10}H_{20}O_2 + H_2O = 190.29$

Colorless or white crystals. M.P. 123° C.
B.P. 258° C. (anhydrous).

0.3% soluble in cold water, 3% soluble in boiling water, 8% soluble in cold alcohol, 30% in boiling alcohol. Poorly soluble in most oils, insoluble in most hydrocarbons (Terpenes, etc.).

Faint, balsamic-piney, camphoraceous, sweet odor. A highly refined, freshly prepared material has very little odor.

Bitter taste in concentrations higher than 40 ppm.

The title material has practically no application in perfumes or flavors as such, but it is briefly mentioned in this work because of its close relationship to the Terpineols, and because it has at one time been used in pharmaceutical praxis for treatment of Tuberculosis. It is still recognized as a mild bactericide.

Since the material is an intermediate in the making of Terpineol from *alpha*-Pinene, a step which is occasionally by-passed, the title material is generally available from manufacturers of Terpineol using that process.

Prod.: from *alpha*-Pinene or Turpentine oil by treatment with dilute sulfuric acid.

It has also been manufactured in the U.S.A. from Pine Oil by acid treatment.

67-516; 67-576; 87-125; 100-1017;

## 2881: TERPINOL

Not a well-defined, single chemical.
A product under the title name is available in Europe and occasionally in the U.S.A., mainly from suppliers of pharmaceutical materials.

The material is a colorless oily liquid.
Sp.Gr. 0.88 and B.P. 168° C. (with a range below and above), insoluble in water, soluble in alcohol and oils.

Sweet, slightly medicinal-camphoraceous-piney odor of moderate tenacity. The sweetness is related to an anisic type of sweetness, the medicinal notes almost cineolic, but not as light or volatile, rather subdued.

The taste is pleasant at concentrations lower than 50 ppm, but bitter at concentrations higher than 200 ppm.

The material is still used in many countries as active ingredient in Licorice-based, small throat-lozenges, with a possible antiseptic and expectorant effect. It is perhaps not surprising, since Terpin hydrate has been used in treatment of Tuberculosis many decades ago.

The title material represents the complete or almost complete composition of fractions from a simple rectification of the reaction mixture obtained by acid hydrolysis of Terpin hydrate, or by simple treatment of Terpin hydrate with dilute sulfuric acid.

It is also obtained as a rectified product from the crude Terpineol reaction mixture ("European type manufacture").

In other words, it contains:
several Terpineol isomers, ($C_{10}H_{18}O$-materials)
Terpinolene,
Terpinene ($C_{10}H_{16}$-materials)
Dipentene

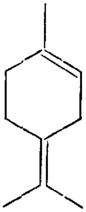
possibly *iso*-Borneol, traces of Cineole, etc.

The material is also briefly mentioned to avoid confusion with Terp*ineol*.

88-54; 100-1018;

## 2882: TERPINOLENE

*para*-Mentha-*1,4(8)*-diene.
*para*-Mentha-*2,4(8)*-diene (the isomer, included in this monograph).
*1,4(8)*-Terpadiene.
"Tereben" and "Terpinene" are old names, used for mixtures, primarily consisting of Terpinolene and *iso*-Terpinolene.
The commercial material is not always a well-defined, single chemical.



$C_{10}H_{16} = 136.24$

Colorless or very pale straw-colored, oily liquid. B.P. 184° C. (polymerizes easily). Sp.Gr. 0.86.

Insoluble in water, soluble in alcohol and oils.

Sweet-piney, oily and relatively pleasant odor of moderate to poor tenacity. Not nearly as harsh as Pinene, often slightly anisic in its sweetness, and generally free from Turpentine-like notes.

Commercial products still sold under names, such as "Tereben" and "Terpinene", often contain significant amounts of *para*-Cymene, Camphene, Dipentene, etc. apart from Terpinolene, the main component.

The title material is used in fragrances for household products, mostly in Pine fragrances, in cleansers, in deodorizers, "reodorants", masking agents, etc. for industrial purposes.

The better grades Terpinolene, often redistilled by the user, are also used in flavor compositions, mainly in Citrus and fruit blends. The concentration may be about 15 to 60 ppm in the finished product. The material is particularly suitable for Lime flavors.

G.R.A.S. F.E.M.A. No.3046.

Prod.:

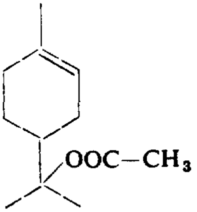
1) by alcoholic sulfuric acid treatment of Pinene.
2) by fractionation out of Wood Turpentine or Sulfate Turpentine, also from ordinary Turpentine oils.
3) as a by-product in the manufacture of Terpineol from Pinene.

31-9; 34-806; 67-508; 87-75;
The Glidden Co., data sheet.

## 2883: TERPINYL ACETATE

*para*-Menth-*1*-en-*8*-yl acetate.

Commercial material is mostly *alpha*-Terpinyl acetate, while the *beta*-isomer is preferred by some perfumers.



$C_{12}H_{20}O_2 = 196.29$

Colorless liquid. Sp.Gr. 0.96. B.P. 220° C.

Almost insoluble in water, soluble in alcohol and oils.

Mildly herbaceous, sweet and refreshing odor of spicy Bergamot-Lavender type, with variations into piney notes according to quality of the ester. Overall much weaker than Linalyl acetate, but of slightly better tenacity.

Warm-herbaceous, mildly spicy taste in concentrations near 40 ppm. The title ester is widely used in common perfumery for low-cost fragrances of the Lavender, Bergamot, Fougère, Citrus, Pine, Spice and other types. In spite of its apparent weakness of odor as compared to Linalyl acetate, it is often preferred in soap because it is far more stable to alkali than Linalyl acetate is.

The ester blends very well with Citronella oil and similar materials for low-cost fragrances for household products, masking odors, etc. However, its role as a substitute for Linalyl acetate and an adulterant in Lavender/Lavandin/Bergamot oils is more or less outdated, partly because of the availability of much more ingenious materials "for the purpose", partly because of the drastic reduction in the cost of Linalyl acetate. The quality of the title ester varies considerably according to the starting materials, the process and the selection of fractions from the rectification of the ester. Most manufacturers have at least two grades of Terpinyl acetate, one being a "perfumery grade", particularly free from piney notes, etc.

The ester finds some use in flavor compositions, in berry complexes, in imitation Lime, Orange, Cherry, Peach Plum, Apricot, and as a minor component of Spice blends for meat flavors. It is often used to "stretch" Cardamom, Origanum, Thyme and other condiment oils.

The concentration in finished products is normally about 1 to 15 ppm, but it may be as high as 260 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.3047.

Prod.: from (*alpha*- or *beta*-) Terpineol by cold Acetylation with Acetic anhydride in presence of Phosphoric acid, or with Sodium acetate and a high-boiling solvent. It is also manufactured by azeotropic esterification of Terpineol with Acetic acid.

Other methods start directly from *alpha*-Pinene.

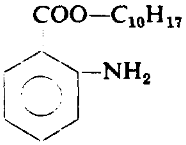
*beta*-Terpinyl acetate is generally considered slightly fresher, more "citrusy" than *alpha*-Terpinyl acetate, but it is not common practise to offer the two isomers individually. It could very well be that perfumers who smell purified *beta*-Terpinyl acetate prefer this isomer because it is purified (and free from Pinene, piney odors, hydrocarbons, etc.) while the commercial "*alpha*-Terpinyl acetate" is not always so carefully purified, because it is the common article.

It has been practised, however, to esterify the discarded alcoholfractions from Terpineol-redistillation in order to make Terpinyl acetate from a low-cost raw material. Obviously, such esters will have an abnormal composition and a different odor.

5-252; 33-503; 90-288; 95-179; 96-214; 103-98; 106-332; 156-329; 156-336; 163-72; 163-238; B-VI-60;

## 2884: TERPINYL ANTHRANILATE

*para*-Menth-*1*-en-*8*-yl-*ortho*-aminobenzoate.
For complete structure: see Terpineol.



$C_{17}H_{23}NO_2 = 273.38$

Colorless or straw-colored oily liquid, solidifying in the cold. Sp.Gr. 1.05.

Insoluble in water, soluble in alcohol and oils.

Musty, heavy, but sweet and Neroli-floral, very tenacious odor. Considerable variations in quality are reflected in this odor picture.

Powerful, sweet-fruity taste in concentrations below 10 ppm, while higher levels tend to produce "harsh-perfumery" flavor.

This ester is occasionally used in perfume compositions, but it is the author's impression that perfumers are generally extremely conservative with respect to Anthranilates, and rarely deviate from the few "big" esters. One must add, however, that the title ester is not very interesting and its fragrance effect is easily achieved or duplicated with more conventional materials.

The title ester is used in variations of Orange blossom, Honeysuckle and other heavy florals, Oriental fragrance types, etc.

It is also used in fruit flavor compositions in concentrations equal to about 1 to 6 ppm in the finished product.

G.R.A.S. F.E.M.A. No.3048.

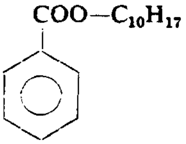
Prod.:

1) from Terpineol and Isatoic anhydride in the presence of minute amounts of Sodium hydroxide.
2) from Methyl anthranilate plus Terpineol-sodium and Terpinyl formate.

5-296; 34-1022; 103-166; 163-72; 163-238;

## 2885: TERPINYL BENZOATE

*para*-Menth-*1*-en-*8*-yl benzoate.
For complete structure – see: Terpineol.



$C_{17}H_{22}O_2 = 258.36$

Colorless or very pale straw-colored, slightly viscous liquid.

Insoluble in water, soluble in alcohol and oils.

Weak, but tenacious, woody-floral, warm odor with a musky undertone.

The title ester has found a little use in perfumery as a fixative and blender in balsamic, Oriental, heavy floral and perhaps Chypre type fragrances. It blends well with Ylang, Sandalwood, Oakmoss, etc. for such purposes, but its contribution to the overall odor is very small.

Prod.: by azeotropic esterification of Terpineol with Benzoic acid in the presence of a Naphthalenesulfonic acid catalyst.

103-131; 163-238; 163-72; 36-176;

## 2886: TERPINYL-n-BUTYRATE

*para*-Menth-*1*-en-*8*-yl-*n*-butanoate.
For complete structure – see: Terpineol.

$C_{10}H_{17}—OOC(CH_2)_2CH_3$

$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. Sp.Gr. 0.94.
B.P. 246° C.

Almost insoluble in water, soluble in alcohol and oils.

Balsamic-floral, sweet and mild, slightly fruity-herbaceous odor of moderate tenacity.

Peculiar fruity taste in concentrations lower than 40 ppm.

This ester is occasionally used in perfume compositions as a modifier in Oriental, Fougère, Rose, Lilac, Lily and other fragrance types, often in combination with the herbaceous oils: Sage, Spike Lavender, Rosemary, etc.

It is also used to a small extent in fruit flavor compositions, e. g. imitation Pineapple and Apricot, fruit complexes, etc.

The concentration in finished products is about 6 to 12 ppm, but it may be as high as 200 ppm in chewing gum.

G.R.A.S. F.E.M.A. No.3049.

Prod.: by azeotropic esterification of Terpineol with *n*-Butyric acid.

5-233; 33-734; 36-176; 90-297; 103-117; 106-336; 163-72; 163-238;

## 2887: TERPINYL-iso-BUTYRATE

*para*-Menth-*1*-en-*8*-yl-*iso*-butyrate.
For complete structure – see: Terpineol.

$C_{10}H_{17}—OOC—CH(CH_3)_2$

$C_{14}H_{24}O_2 = 224.35$

Colorless oily liquid. Sp.Gr. 0.93.
B.P. 242° C.

Almost insoluble in water, soluble in alcohol and oils.

Fruity-floral-herbaceous, refreshing and moderately tenacious odor. More delicate and "clean" than the *n*-butyrate, not as harsh-herbaceous.

Heavy-fruity, nondescript type flavor in concentrations below 40 ppm.

This ester finds a little use in perfume compositions of Rose, Lavender and Geranium types. It is particularly useful in soap perfumes because of its outstanding stability in alkaline media.

Small amounts are used in various fruit flavor compositions, in concentrations equal to about 2 to 15 ppm in the finished products.

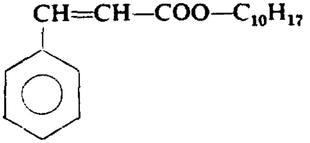
G.R.A.S. F.E.M.A. No.3050.

Prod.: by azeotropic type esterification of Terpineol with *iso*-Butyric acid.

5-233; 90-297; 156-329; 163-72; 163-238;

## 2888: TERPINYL CINNAMATE

*para*-Menth-*1*-en-*8*-yl cinnamate.
For complete structure – see: Terpineol.



$C_{19}H_{24}O_2 = 284.40$

Colorless or pale straw-colored, slightly viscous liquid.
Sp.Gr. 1.03. B.P. 360° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Mild, sweet, floral-balsamic and very tenacious odor, resembling Perubalsam or Tolubalsam, and terpeneless Nutmeg to a certain degree. The immediate impression is that of a weak odor.

Heavy-fruity, mildly spicy taste in concentrations below 20 ppm.

The title ester is not often offered commercially, but it finds a little use in New-Mown-Hay, Fougère, Oriental bases, Muguet variations (Linalyl cinnamate is preferred by far), etc.

It blends very well with Labdanum for such purposes.

Traces of the ester are used in fruit flavor compositions, sometimes in Grape imitation, and in certain Spice complexes.

The concentration used is normally as low as 0.5 to 6 ppm in the finished product.

G.R.A.S. F.E.M.A. No.3051.

Prod.:

1) by azeotropic type esterification from Terpineol and Cinnamic acid.
2) from Methyl cinnamate, Sodium-terpineol and Terpinyl formate (or Terpinyl acetate).

34-484; 36-176; 103-148; 159-644; 163-72; 163-238;

## 2889: TERPINYL FORMATE

*para*-Menth-*1*-en-*8*-yl formate.
For complete structure - see: Terpineol.

$C_{10}H_{17}{-}OOC{-}H$

$C_{11}H_{18}O_2 = 182.27$

Colorless liquid. Sp.Gr. 0.99. B.P. 213° C.

Very slightly soluble in water, soluble in alcohol and oils.

Fresh, floral-citrusy, tart-herbaceous, semi-dry odor of moderate to poor tenacity.

Peculiar "astringent-dry" fruity taste, bitter in concentrations higher than 20 ppm.

This ester is quite well known, but often remains unused on the perfumer's shelf, resulting in the material becoming sour or decomposed. Formates are generally very interesting odorants, and provided they are of high chemical purity, they will normally keep well on the shelf.

The ester finds some use in Citrus-colognes, in support of Neroli notes, Lavender-Bergamot-notes, green notes, etc. It is also used in certain topnote compositions with Citrus oils and "green" materials.

The title material is used in certain types of fruit flavor composition, mainly in berry-types and in "Bitters".

The concentration will be about 0.5 to 10 ppm in the finished product.

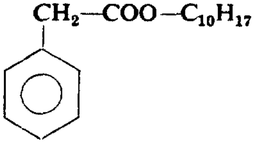
G.R.A.S. F.E.M.A. No.3052.

Prod.: by cold Formylation of Terpineol, using Formico-Acetic anhydride.

5-246; 36-176; 90-286; 103-86; 156-336; 163-72; 163-238;

## 2890: TERPINYL PHENYLACETATE

*para*-Menth-*1*-en-*8*-yl-*alpha*-toluate.
For complete structure - see: Terpineol.



$C_{18}H_{24}O_2 = 272.39$

Colorless or very pale straw-colored, slightly viscous liquid, solidifying in the cold. Sp.Gr. 1.02. B.P. 322° C.

Insoluble in water, soluble in alcohol and oils.

Relatively weak, but rather heavy, sweet-floral and very tenacious odor of Rose-Lilac-Honey complex, with the usual variations according to the purity of the ester (and the method of production).

Although rarely found in the price lists, the ester is occasionally used in Gardenia, Honeysuckle, Narcisse, Rose, Neroli, Lily and Lilac bases, mainly as a fixative and blender.

Prod.: by azeotropic type esterification of Terpineol with Phenylacetic acid. With proper catalyst, this method produces a fairly high-grade material.

5-271; 34-246; 36-176; 103-141; 163-72; 163-238;

## 2891: TERPINYL PROPIONATE

*para*-Menth-*1*-en-*8*-yl propionate.
For complete structure – see: Terpineol.

$C_{10}H_{17}$—OOC—$C_2H_5$

$C_{13}H_{22}O_2 = 210.32$

Colorless oily liquid.
Sp.Gr. 0.95. B.P. 240° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-herbaceous, mildly fruity-piney, refreshing odor of moderate tenacity.

Nondescript fruity taste in concentrations below 20 ppm. Some resemblance to Pear.

The title ester has acquired fame as a modifier for Lavender and Bergamot but it is really no match for Linalyl acetate or Ethyl linalyl acetate except that the Terpinyl propionate is very stable in alkaline media. It is therefore often used in soap, where its low cost is also appreciated.

For Pine variations, Citrus colognes, Lavender, Sage and other herbaceous fragrances, Fougères, etc. it is a common ingredient when price puts a limit to the perfumer's creative activity.

The ester finds a little use in fruit complex flavor compositions, mainly in Citrus fruits, Lime, Spice (Cardamom) etc. The concentration will be about 1 to 10 ppm in the finished product.

G.R.A.S. F.E.M.A. No.3053.

Prod.:

1) from Terpineol and Propionic anhydride with a neutral diluent under reflex. Terpinyl propionate has also been used as the diluent.
2) by azeotropic type esterification of Terpineol with Propionic acid.

5-232; 14-133; 17-394; 31-285; 33-622; 36-176; 38-665; 90-296; 103-108; 106-334; 156-336; 163-72; 163-238;

## 2892: TERPINYL-n-VALERATE

*para*-Menth-*1*-en-*8*-yl-*n*-pentanoate.
For complete structure – see: Terpineol.

$C_{10}H_{17}$—OOC$(CH_2)_3CH_3$

$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid.
Sp.Gr. 0.93. B.P. 256° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, herbaceous-piney, almost Ambre-like, Citrus-incense type odor of moderate tenacity.

This ester, although rarely offered commercially, finds a little use in perfume compositions for novel notes in Men's fragrances, as a modifier in Juniperberry-Ambre-Cypres notes, incense-notes, or balsamic-floral and various herbaceous fragrance types.

It blends very well with Labdanum, Lavender, Styrax, Oakmoss, Amylsalicylate, Sage, etc. for such purposes.

Prod.: by azeotropic esterification of Terpineol with *n*-Valeric acid.

33-933; 90-299; 156-336; 163-72; 163-239;

## 2893: TERPINYL-iso-VALERATE

*para*-Menth-*1*-en-*8*-yl-*beta*-methylbutyrate.
For complete structure - see: Terpineol.

$C_{10}H_{17}—OOC—CH_2—CH(CH_3)_2$

$C_{15}H_{26}O_2 = 238.37$

Colorless oily liquid.
B.P. 248° C. Sp.Gr. 0.93.

Almost insoluble in water, soluble in alcohol and oils.

Peculiar sweet-piney, floral-incense-like, citrusy odor of moderate tenacity. Less herbaceous, more floral-fruity than the *n*-valerate.

Heavy-fruity, sweet taste in concentrations near 20 ppm, but rather piney-fruity at higher levels.

This ester finds limited use in perfume compositions of the Chypre, Fougère, Bruyère, "Tabac", Opopanax, Lavender and various herbaceous types. It blends very well with the Olibanum-Opopanax-Labdanum-Styrax resinoids, and with the heavier herbaceous materials.

It is also used to a minor extent in flavor compositions, in various fruit complexes, and in Tobacco flavorings.

The concentration in finished products is normally about 0.5 to 10 ppm.

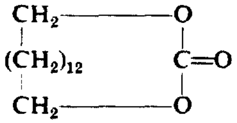
G.R.A.S. F.E.M.A. No.3054.

Prod.: by azeotropic type esterification of Terpineol with *iso*-Valeric acid.

5-239; 36-176; 103-125; 163-72; 163-238;

## 2894: TETRADECAMETHYLENE CARBOXYLATE

Tetradecamethylene carbonate.
NOTE*) "Hexadecamethylene cyclocarbonate (misleading name).



$C_{15}H_{28}O_3 = 256.39$

Colorless, slightly viscous liquid, solidifying in the cold. M.P. 31° C. B.P. slightly higher than 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, sweet-musky, mildly animal odor with considerable resemblance to the odor of Cyclopentadecanolide, and with excellent tenacity.

The title "macrocylic musk" is not a common commercial article, but it has been prepared by various larger houses for private use in perfumes, also for experimental comparison with Cyclopentadecanolide, which has achieved reputation as the "standard", against which almost all other musks are evaluated.

The title material is a very useful musk, but not yet very inexpensive. It has a tenacity almost comparable to that of Cyclopentadecanolide, but does not seem to compare well against this material with respect to olfactory effect on the skin - the "wearability". And it does not produce the desirable musk effect at the same low level of concentration as does Cyclopentadecanolide.

It is interesting to note that the subject musk is an empirical isomer and very close relative of the successful Oxahexadecanolide musks (see monographs).

If new synthetic methods, or improved technique can produce the title material at a competitive cost, there is good reason to believe that it can enter the shelves in the perfume laboratories and replace or supplement the currently popular musks.

Prod.: from Tetradecamethylene glycol and Butylcarbonate with Sodium, followed by decarboxylation by heat.

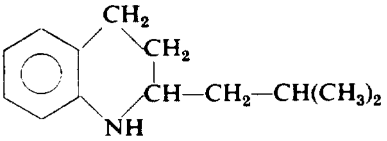
NOTE*) This material has been mentioned in literature and suggested for use as a macrocyclic type musk with Civettone-like effect. It has also been stated that 17 members in the ring (Carbon- and Oxygen-atoms total) favor such odor type. However, the author is not aware of any such chemical being commercially marketed. It is possible that confusion with Hexadecamethylene carbonate exists.

The above structure describes a macrocyclic carbonate with a total of 15 Carbon atoms, and a material of that structure has a musklike odor.

31-127; 156-251; 156-261; 159-439; 86-58;

## 2895: TETRAHYDRO-iso-BUTYLQUINOLINE

The product, occasionally available commercially, consists mainly of:
*1,2,3,4*-Tetrahydro-*alpha-iso*-butylquinoline.
while the *5,6,7,8*-Tetrahydro-isomer may or may not be present in smaller amounts.



$C_{13}H_{19}N = 189.30$

Colorless or very pale straw-colored, oily liquid. B.P. 261° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-woody, nut-like, earthy and mildly medicinal-leathery odor of considerable tenacity.

This material, rarely offered commercially under its proper chemical name, has found some use in perfume compositions, e. g. in bouquetting of Vetiver notes, in artificial Vetiver oils, in Chypre and Tabac-type fragrances, and in many novel fragrances, often with Oakmoss, Vetiver, Coumarins and musks.

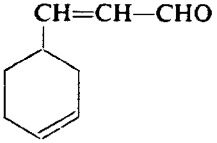
It is interesting from a physical point of view in that it has a higher boiling point than the unsaturated (and better known) material, *iso*-Butylquinoline (see monographs).

Prod.: by hydrogenation of *alpha-iso*-Butylquinoline with Nickel catalyst.

69-643;

## 2896: TETRAHYDRO CINNAMIC ALDEHYDE

*3*-(Cyclohex-*3*-en-*1*-yl)-propen-*2*-al-*1*.



$C_9H_{12}O = 136.20$

Colorless or pale yellowish oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-green, leafy, delicately creamy odor, in dilution floral, and tenacious.

The title aldehyde, commonly referred to under the title name, was developed many years ago in continuation of the search for interesting aldehydes from the Claisen reaction, by which Cinnamic aldehyde had been produced. It was also based upon a new method of obtaining Cyclohexene aldehydes and homologues of same.

The subject material has found some application in perfumery, and so has the Cyclohexene carboxaldehyde from which it is made. The parent cyclic aldehyde has a powerful green-leafy odor, and it was interesting to see what type odor could be obtained by the Claisen condensation.

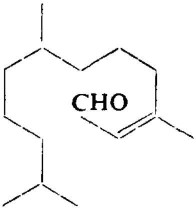
Although rarely offered under its proper chemical name, this material is still used in various perfume specialties and bases for its refreshing, green note, sometimes useful in Citrus compositions, but also used in Chypres, Fougères, etc. in combination with Oakmoss, Lavender, etc.

Prod.: from Acrolein and Butadiene to make Cyclohex-*3*-enealdehyde. By condensation (Claisen) with Acetaldehyde the title material is obtained.

67-190;
Firmenich patent 1929 No. 672025, French.

## 2897: TETRAHYDRO FARNESAL

*3,7,11*-Trimethyl-*2*-dodecen-*1*-al.
*2,6,10*-Trimethyl-*10*-dodecen-*12*-al (sometimes called).



$C_{15}H_{28}O = 224.39$

Almost colorless or pale straw-colored, oily or slightly viscous liquid. Polymerizes in air, becoming yellowish, more viscous, and changing its odor.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, very sweet, fruity-floral and tenacious odor.

The title aldehyde, not a very common article, and rarely offered under its proper chemical name, has found a little use in perfumery. Several very closely related aldehydes are used more commonly and are often considered more stable, therefore preferred.

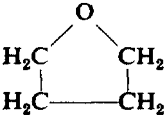
As a minor component in topnote compositions, in Muguet, Lily, Peony, Rose, Cyclamen, Magnolia, etc., it may introduce a pleasant, fresh and powerful, tenacious note of excellent blending properties.

Prod.: by regulated hydrogenation of Farnesal.

2-1008; 89-125;
See also monographs:
Trimethyl undecylenic aldehyde, and
Trimethyl undecylic aldehyde.

## 2898: TETRAHYDROFURAN

Tetramethylene oxide.
Diethylene oxide.



$C_4H_8O = 72.11$

Colorless mobile liquid.
B.P. 66° C. Sp.Gr. 0.89.

Miscible with water and alcohol, soluble in most oils.

The material is flammable and very easily oxidized. The oxidized material is extremely explosive.

Penetrating, sweet-gassy and warm, bread-like odor. Unpleasant in its diffusive power and pungency. Very poor tenacity.

The title material is briefly mentioned in this work because it is the parent material for a large number of very useful perfume and flavor chemicals. It is also an important solvent for the perfumery and flavor research chemists.

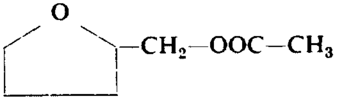
The material as such is probably not used in perfumes or flavors. Many of the derivatives are used in reconstituted Coffee, Caramel, Maple and similar flavors.

Prod.:
1) from *1:4*-Butane diol by dehydration with Phosphoric acid at high temperature.
2) a number of methods start from Furfural, via Furan.

31-150; 69-163; 100-1023; B-XVII-10;

## 2899: TETRAHYDRO FURFURYL ACETATE

Tetrahydro-*2*-furyl methylacetate.



$C_7H_{12}O_3$ = 144.17

Colorless liquid. Sp.Gr. 1.06. B.P. 196° C.

Miscible with water, alcohol and oils.

Mild, fruity, Acetone-ethereal odor of moderate to poor tenacity.

Sweet, ethereal and deep-fruity taste at concentrations below 40 ppm.

The title ester is used as a solvent industrially, but it finds only very little use in perfumery.

It finds a little use in flavor compositions as part of imitation Maple, Honey and various fruit flavors, e. g. Apricot.

The concentration used is about 2 to 20 ppm in the finished product.

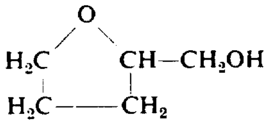
G.R.A.S. F.E.M.A. No.3055.

Prod.: by azeotropic esterification of Tetrahydrofurfuryl alcohol with Acetic acid.

33-500; 155-598; 163-239; B-XVII-107, zweiter Ergänzungsband.

## 2900: TETRAHYDRO FURFURYL ALCOHOL

Tetrahydro-*2*-furancarbinol.
Tetrahydro-*2*-furanmethanol.
Tetrahydro-*2*-furylmethanol.
THFA.



$C_5H_{10}O_2$ = 102.14

Colorless liquid. B.P. 179° C. Sp.Gr. 1.05.

Miscible with water, alcohol and oils.

Mild, warm, oily-caramellic odor of moderate to poor tenacity.

This material was introduced on the chemical solvent market many years ago, and quickly found uses in the cosmetic field, e. g. as a solvent for lipstick-colors. A question about its physiological effect and statements that the material may not be absolutely harmless resulted in many derivatives being devloped from this alcohol.

The esters are considered practically harmless, but they are poorer solvents. A number of esters are used in flavors, see the following monographs.

There is very little use for the title alcohol as such in perfume compositions. Its low boiling point and not extremely attractive odor are factors speaking against the wider use of the alcohol.

It finds some use in flavor compositions, mainly of the Coffee and Nut type, but concentrations are normally very low, e. g. between 0.03 and 1 ppm, but in certain types of imitation Coffee flavor it may be about 20 ppm in the finished product.

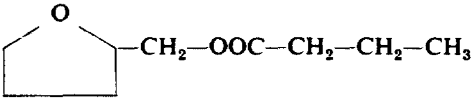
G.R.A.S. F.E.M.A. No.3056.

Prod.:
1) from Furfural via *2*-Furanmethanol by hydrogenation with Raney-Nickel catalyst.
2) The alcohol has also been prepared by destructive hydrogenation of Lignin.

69-165; 100-1024; 155-598; B-XVII-106, zweiter Ergänzungsband.

## 2901: TETRAHYDROFURFURYL-n-BUTYRATE

Tetrahydro-2-furylmethyl-*n*-butanoate.



$C_9H_{16}O_3$ = 172.23

Colorless liquid. Sp.Gr. 1.01. B.P. 227° C.

Insoluble in water, soluble in alcohol, miscible with oils.

Heavy, sweet-fruity odor of Apricot-Pineapple type, moderate tenacity.

Sweet-fruity taste at concentrations below 40 ppm, but rather pungent and unnatural at higher levels.

The title ester has found some use in fruit flavor compositions, mainly as a fixative for the more volatile esters (Butyl butyrate, etc.), and as a modifier in general. It can not be used at the same high levels as used for the conventional "fruit esters", because it is deficient in natural character, yet it has an overall pleasant effect at low levels, and is quite versatile then.

Concentrations in finished products are about 1 to 15 ppm.

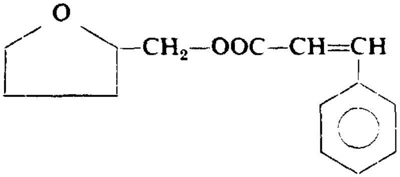
Prod.: by azeotropic esterification of Tetrahydrofurfuryl alcohol with *n*-Butyric acid.

G.R.A.S. F.E.M.A. No.3057.

26-684;

## 2902: TETRAHYDRO FURFURYL CINNAMATE

Tetrahydro-2-furyl methyl cinnamate.



$C_{14}H_{16}O_3$ = 232.28

Colorless, slightly viscous liquid.
Sp.Gr. 1.11. B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Mild, sweet and very tenacious, balsamic-winey, slightly spicy odor.

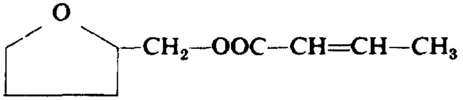
The title material has found a little use in perfume compositions, since it combines very pleasantly with Labdanum notes and other sweet-herbaceous fixative materials, Ambre-notes, etc.

The author is not aware of any significant use of this ester in flavor compositions.

Prod.: by azeotropic esterification of Tetrahydrofurfuryl alcohol with Cinnamic acid.

## 2903: TETRAHYDRO FURFURYL CROTONATE

(Tetrahydro-2-furylmethyl)-2-butenoate.
Tetrahydro-2-furylmethyl-*alpha*-crotonate.



$C_9H_{14}O_3$ = 170.21

Colorless oily liquid.
B.P. 242° C. Sp.Gr. 1.05.

Almost insoluble in water, soluble in alcohol, miscible with oils.

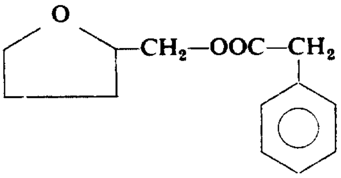
Warm, caramellic-herbaceous, mildly balsamic odor, in dilution almost floral in its balsam-notes. Moderate tenacity.

The title ester is very rarely offered under its proper chemical name, but finds some use in perfume compositions as an "undertone" and occasionally as part of the less volatile base in a topnote composition. It will support herbaceous and balsamic-floral notes, Ylang, Labdanum, Rose, etc. and blends very well with Juniper berry oil notes in Ambre compositions.

Prod.: by azeotropic esterification of Tetrahydrofurfuryl alcohol with 2-Butenoic acid (*alpha*-Crotonic acid).

## 2904: TETRAHYDRO FURFURYL PHENYLACETATE

Tetrahydro-2-furyl-methyl-*alpha*-toluate.



$C_{13}H_{16}O_3 = 220.27$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol miscible with oils.

Mild and heavy-sweet, very tenacious Honey-Rose type odor with a Raspberry-fruity undertone.

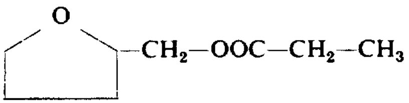
This ester is occasionally used in perfume compositions as a modifier in Oriental and heavy floral fragrance types. Its tenacity and good blending abilities make it a relatively useful material, although it is not regularly available from the manufacturers of perfume chemicals.

It gives interesting effects in Rose bases with heavy fruity notes, such as Ionones, Ethyl methyl phenyl glycidate, Oxyphenylon, Palatone, etc.

Prod.: by azeotropic esterification of Tetrahydrofurfuryl alcohol with Phenylacetic acid.

## 2905: TETRAHYDRO FURFURYL PROPIONATE

Tetrahydro-2-furyl-methyl propionate.



$C_8H_{14}O_3 = 158.20$

Colorless liquid. Sp.Gr. 1.04. B.P. 207° C.

Poorly soluble in water, miscible with alcohol and oils.

Caramellic-sweet, fruity and soft-oily odor of moderate tenacity.

Sweet, fruity-caramellic, but not burnt, taste in concentrations below 40 ppm. More fruity, less caramellic at higher concentrations.

The title ester has found some use in flavor compositions for imitation Rum, Honey, Chocolate, Maple and occasionally in certain Nut composition-flavors.

The concentration used is equivalent to about 1 to 20 ppm in finished products.

The author is not aware of any significant use of this ester in perfume compositions, but it seems to have quite interesting effect along with Linalool in Ylang compositions.

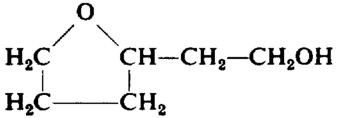
G.R.A.S. F.E.M.A. No.3058.

Prod.: by azeotropic esterification of Tetrahydrofurfuryl alcohol with Propionic acid.

26-684;

## 2906: 2-(TETRAHYDROFURYL)-ETHANOL-2

Tetrahydrofuran ethylalcohol.
*alpha*-2-Hydroxyethyl furan.



$C_6H_{12}O_2 = 116.16$

Colorless oily liquid. B.P. 184° C. Sp.Gr. 1.03.

Very slightly soluble in water, miscible with alcohol and oils.

Sweet, oily, warm and remotely caramellic-floral odor of moderate to poor tenacity. In dilution also winey.

This material has been suggested for use in perfume compositions, and it has at times a pleasant mellowing effect upon topnote compositions for fruity floral creations. It blends very well with Labdanum, Clary Sage, Rose, soft fruity notes, and with moderate amounts of Ionones. It finds some use in perfume specialties and bases.

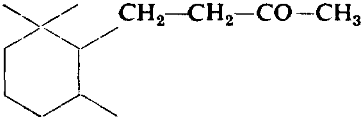
Prod.:

1) from Furfural and Methyl chloroacetate via the glycidic ester to 2-Furylacetaldehyde which is hydrogenated and reduced to the title material.
2) from *beta-2*-Furylethanol by hydrogenation. The unsaturated alcohol is obtained by Bouveault-Blanc reaction upon Ethyl-2-furylacetate.

69-166;

## 2907: TETRAHYDRO IONONE

*4*-(*2,6,6*-Trimethylcyclohexyl)-butan-*2*-one.



$C_{13}H_{24}O = 196.34$

Almost colorless oily liquid.
B.P. 235° C. Sp.Gr. 0.90.

Practically insoluble in water, soluble in alcohol and oils.

This ketone is rarely found in the perfume laboratory. It seems to be much less common than Tetrahydro-pseudo-ionone, or other hydrogenated Pseudo-ionones.

The title material has an unquestionable Cedarwood-like odor, and that is, of course, not very exciting. It does not have the soft or velvety notes of the Ionones, nor does it display any of the oily-floral notes of hydrogenated Pseudo-ionones.

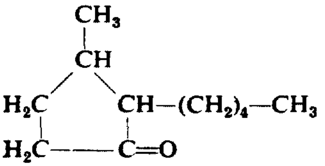
Apart from occasional use in special variations of the Ionone themes and as a supporting note in perfumes with Ambre emphasis, the title material has very little importance.

Prod.: by controlled hydrogenation of Ionone (*alpha*- or *beta*-) with a Platinum catalyst. Complete hydrogenation may lead to the alcohol (Tetrahydro ionol).

5-97; 31-94; 89-385; 163-240; 163-379;

## 2908: TETRAHYDROJASMONE

*3*-Methyl-*2*-(*n*-pentyl)-cyclopentanone-*1*.
Hexahydro pyrethrone.
Methyl amyl cyclopentanone.
For the isomer: Methyl-*iso*-amyl cyclopentanone, see monograph under that name.



$C_{11}H_{20}O = 168.28$

Colorless or almost colorless oily liquid.
Sp.Gr. 0.89. B.P. 214° C.

Practically insoluble in water, soluble in alcohol and oils.

Fruity-sweet, in dilution somewhat floral odor of moderate to poor tenacity. The fruity notes are much more pronounced in this ketone than in Dihydrojasmone, and the floral notes not nearly as warm-herbaceous.

The title ketone, a result of meticulous research into the derivatives of Cyclopentanone and Cyclopentenone, related to Jasmone, has found some use in perfumery. However, it is generally agreed that it is not nearly as suitable for Jasmin notes as are the *iso*-Jasmones, the Dihydrojasmones, and even the *iso*-amyl-isomer of the title material. Only the relatively low cost kept this ketone in use, but the cost is no longer competitive with that of the named Jasmone materials.

For pronounced fruity Jasmin base types, the subject ketone may still be useful although not always powerful enough.

Prod.:

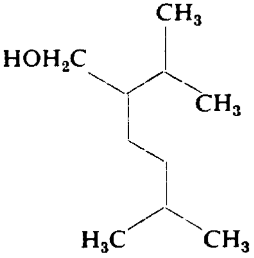
1) from Undecane-diol.
2) from Cyclopentanone by condensation with *n*-Valeric aldehyde, followed by hydrogenation of the unsaturated ketone.

Samples: Compagnie Parento, Inc.

5-152; 5-154; 156-223; 163-72; 163-240; 163-379;
See also monograph: *3*-Methyl-*2*-*iso*-amyl cyclopentanone.

## 2909: TETRAHYDRO LAVANDULOL

"Lavandor".
*2,6*-Dimethyl-*5*-hydroxymethyl heptane.
*2*-*iso*-Propyl-*5*-methylhexanol-*1*.
*5*-Methyl-*2*-*iso*-propylhexanol-*1*.
*2,4*-Di-*iso*-propyl-*1*-butanol.



$C_{10}H_{22}O = 158.29$

Colorless liquid. B.P. 206° C.

Very slightly soluble in water, soluble in alcohol and oils.

Mild, sweet-herbaceous and discretely floral odor of moderate to poor tenacity. The odor is suggestive of Lavender, Clary Sage, Bergamot, etc.

This alcohol was introduced shortly after World War II by a large German chemical company, in which the material had already been developed many years earlier.

It represents in a way the beginning of the availability to the perfumer of the more "sophisticated" Lavender materials. Until then, the perfumer had had to rely almost exclusively upon Linalool and its esters as a base for Lavender/Lavandin oils.

Since Lavandulol – a "wanted" material for Lavender reconstruction – was difficult to synthesize, the Tetrahydrolavandulol and its esters were marketed at a very favorable price in 1950.

The importance of Tetrahydrolavandulol never grew very high, and it is again dwindling as a number of new Lavender materials become available and since Linalool/Linalylacetate are now priced well below the cost of Lavandin oil.

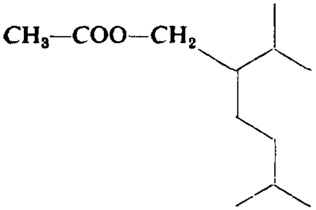
The title material has a more floral and less woody odor than Linalool, and is therefore more versatile. In this respect is resembles Tetrahydrolinalool, but it lacks the softness of the latter.

Prod.: Originally from Methylheptenone, but newer methods were developed until Lavandulol was synthesized directly, and the title material could be obtained by hydrogenation.

87-577; 163-240; 163-379;
Sample: Badische Anilin- und Soda-fabriken, A.G. (Germany).

## 2910: TETRAHYDRO LAVANDULYL ACETATE

"Lavandor acetate".
*2*-*iso*-Propyl-*5*-methylhexan-*1*-yl acetate.
*5*-Methyl-*2*-*iso*-propylhexan-*1*-yl acetate.



$C_{12}H_{24}O_2 = 200.32$

Colorless liquid. Sp.Gr. 0.87. B.P. 212° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, fruity-herbaceous odor, suggestive of Lavender, Bergamot and Clary Sage, yet warmer and more herbaceous than Linalyl acetate.

This ester has had use in perfumery as a modifier for Linalyl acetate in Lavender, Lavandin, Bergamot and other compositions. It became available at a time of very high cost of Linalyl acetate and almost non-existence of other Lavender esters.

However, it has lost much of its importance in view of the better availability of Lavandulol esters, and the much lower cost of Linalyl esters.

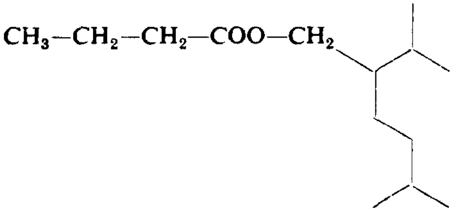
If it were available at a competitive cost, the title material could undoubtedly still be used in Lavender-Lavandin compositions, soap perfumes, and in general cosmetic fragrance work as a modifier and variant of the Lavender type chemicals of excellent stability.

Prod.: by Acetylation of Tetrahydrolavandulol. This alcohol is a primary alcohol and therefore esterified much safer than Linalool.

163-240;
Sample: Badische Anilin- und Sodafabriken, A.G. (Germany).

## 2911: TETRAHYDROLAVANDULYL-n-BUTYRATE

"Lavandor butyrate".
*2*-*iso*-Propyl-*5*-methylhexan-*1*-yl-*n*-butanoate.
*5*-Methyl-*2*-*iso*-propylhexan-*1*-yl-*n*-butanoate.



$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid.
Sp.Gr. 0.86. B.P. 224° C.

Practically insoluble in water, soluble in alcohol and oils.

Very sweet, heavy, fruity-herbaceous odor of moderate tenacity. The fruity-herbaceous notes have some resemblance to Clary Sage, while the deep-sweet fruitiness is somewhat Pineapple-like.

This ester has at one time been used in perfume compositions as a modifier for Linalyl butyrate, and as a fruity-herbaceous ester for general use.

Since the cost of Linalyl butyrate has been brought down, and the availability of other "Lavender" chemicals has improved, the interest in the title material has dwindled considerably.

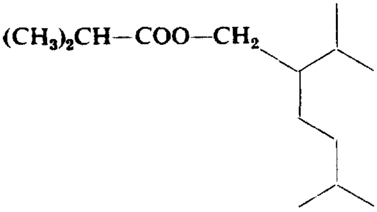
The subject ester has some advantage in being very stable and in the fact that it can be produced in a state of very high purity.

Prod.: from Tetrahydrolavandulol and *n*-Butyric acid.

163-240;
Sample: Badische Anilin- und Sodafabriken, A.G.

## 2912: TETRAHYDRO LAVANDULYL-iso-BUTYRATE

"Lavandor-*iso*-butyrate".
*2*-*iso*-Propyl-*5*-methylhexan-*1*-yl-*iso*-butanoate.
*5*-Methyl-*2*-*iso*-propylhexan-*1*-yl-*iso*-butanoate.



$C_{14}H_{28}O_2 = 228.38$

Colorless oily liquid.
B.P. 220° C. Sp.Gr. 0.86.

Practically insoluble in water, soluble in alcohol and oils.

Fresh and sweet, fruity-herbaceous odor of moderate to poor tenacity. Fresher and more fruity than the *n*-Butyrate, but not as natural-herbaceous.

This ester has been used in perfume compositions some years ago, but it has lost most of its importance by the appearance of many other Lavender-materials at low cost.

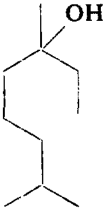
Although the ester is very stable and suitable for soap perfumes, it will not be able to compete with modern, low-cost chemicals of similar odor type, unless its cost is brought to the same level.

Prod.: from Tetrahydrolavandulol and *iso*-Butyric acid.

163-240;
Sample: Badische Anilin- und Sodafabriken, A.G. (Germany).

## 2913: TETRAHYDRO LINALOOL

*3*,*7*-Dimethyloctanol-*3*.



$C_{10}H_{22}O = 158.29$

Colorless oily liquid. Sp.Gr. 0.83.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-oily, delicately floral odor, less green-woody than Linalool, more floral and powdery, sweet-dry odor.

Pleasant citrusy-floral taste in concentrations below 10 ppm. Concentrations higher than 20 ppm tend to appear "perfumey".

This alcohol has been known for many decades, but was only brought on the perfume chemicals market some 10 years ago. After many years of rather unsuccessful existence, the material has finally caught the interest of perfumers to a greater extent, and the price of the title material has reached a more attractive level.

As a major component in delicate floral fragrance types, Muguet, Lily, Lilac, Mimosa, variations of Rose and Jasmin, etc. it has repeatedly confirmed its pleasant effects and good stability.

It is also used in Lavender compositions, Chypres, Fougères, etc. as a modifier/blender, and its mild odor makes it almost universally applicable.

Traces of the alcohol are used in flavor compositions for imitation Citrus, fruit-complexes, berry flavors and certain Liqueur flavors. The concentration in the finished product will usually be as low as 1 to 6 ppm.

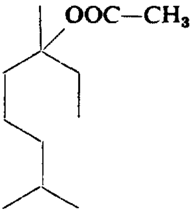
G.R.A.S. F.E.M.A. No.3060.

Prod.: by hydrogenation of Linalool. There are many methods in use and smaller amounts of the title material are also obtained as a by-product in making Dihydro linalool (see monograph).

31-20; 87-531; 106-335; 156-238; 163-72; 163-240; 163-379;

## 2914: TETRAHYDRO LINALYLACETATE

*3*,7-Dimethyloctan-*3*-yl acetate.



$C_{12}H_{24}O_2 = 200.32$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Dry-floral, mildly herbaceous, pleasant odor of moderate tenacity.

This ester has found a little use in perfume compositions, but it has not nearly achieved the position of importance as e. g. Linalyl acetate. It is generally considered weaker, but it is also more floral, and less fruity than Linalyl acetate.

It is therefore not used very frequently in Lavender/Lavandin compositions, or at least not in very large proportions.

Its main use is that of being a modifier in Muguet, a minor ingredient in Bergamot, Lavandin, Lavender, Fougère, etc.

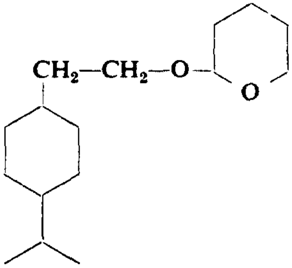
It blends very well with Labdanum, Amylsalicylate, the "rose alcohols" etc. for general creative perfumery.

Prod.: by Acetylation of Tetrahydrolinalool.

Sample: Hoffmann-laRoche, Inc. Aromatic Chemicals Div., Nutley, N.J. (U.S.A.).

## 2915: TETRAHYDRO-2-(para-MENTHAN-7-YL-METHOXY)-PYRAN

*para*-Menthanylcarbinyl tetrahydropyranylether.



$C_{16}H_{30}O_2 = 254.42$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet and warm, oily-herbaceous odor with green-floral notes and moderate to poor tenacity.

The title material has probably not been commercially available under its proper chemical name, but it has been used as part of various bases and specialties. Of the many Pyranylethers known, it is probably one of the less successful ones. One may assume that after being used for more than 10 years, a material will become very well known, copied or in other ways commercially available, if it is particularly interesting, although this is a sort of negative conclusion.

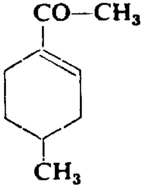
However, most indications point to the fact that the material is more or less obsolete in perfumery.

Prod.: from *2,3*-Dihydro-*gamma*-pyran and Hexahydro-*para*-*iso*-propylphenylethylalcohol by acid hydrolysis. The alcohol is a derivative of Dipentene.

69-840;

## 2916: 1-TETRAHYDRO-$\Delta^1$-*para*-METHYLACETOPHENONE

*1*-Acetyl-*4*-methyl cyclohex-*1*-ene.
Methyl-*para*-methylcyclohexenyl ketone.



$C_9H_{14}O = 138.21$

Colorless or pale straw-colored oily liquid. B.P. 202° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, sweet-herbaceous, rather pungent and "unnatural" odor, unless diluted, when it becomes more pleasant, sweet-herbal.

The title ketone has been suggested for use in perfume compositions as supporting note in various herbaceous bases, such as Lavender, Lavandin, Rosemary, Sage, etc. It performs very well in soap, where its stability and great diffusive power are of use.

Generally, however, the material is not easy to use. It lacks naturalness, and demands very skilled fixation. If it becomes available at very low cost, it could become an important soap perfume material.

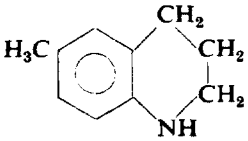
Prod.: from Methyl cyclohexene and Acetylchloride with Aluminum chloride or Stannic chloride.

It has also been synthesized from *1*-Ethynyl-*4*-methylcyclohexan-*1*-ol by rearrangement with Phosphorus pentoxide or Formic acid.

67-216;

## 2917: TETRAHYDRO-para-METHYLQUINOLINE

*para*-Methyl tetrahydroquinoline.
Tetrahydro-*para*-toluquinone.
"Tetraquinone" (Givaudan).
*1,2,3,4*-Tetrahydro-*6*-methylquinoline.
"Civettal" cryst.
"Zibethal".
"Ziberthine".



$C_{10}H_{13}N = 147.22$

Colorless or pale amber-colored, needle-like crystals. M.P. 38° C. B.P. 265° C.

Slightly soluble in water, soluble in alcohol and oils.

Very powerful and tenacious, sweet-animal odor with Honey-like undertone. Floral notes are perceptible upon extreme dilution of the material, but the undiluted quinoline has a rather unpleasant, Civet-like odor.

This material is one of the most frequently used quinoline derivatives in perfumery. In artificial Civet or Civet bases, as a fixative in floral, balsamic, Oriental or Ambre-like fragrances, as a fixative in Honey or Tabac-bases, it is almost a standard ingredient, although always in discrete proportions.

It is also used as a modifier for the excellent, but often neglected Tetrahydro-2-methylquinoline (Hydroquinaldine) in Lilac bases, where it adds not only fixation, but also depth, warmth and very natural character to that type of floral note.

The title material also blends well with Amylcinnamic aldehyde for variations in the Jasmin theme, Tuberose, Gardenia and many other heavy or "exotic" florals. With Phenylacetic acid, Opopanax, Sandalwood and Cinnamates, it may contribute fixation and background for "Oriental" fragrances, etc.

Prod.: from *6*-Methylquinoline hydrochloride by reduction with nascent Hydrogen, followed by neutralization.

Also with Hydrogen and a Nickel catalyst.

The Methylquinoline is usually obtained by a Skraup's synthesis.

5-308; 37-939; 68-643; 106-336; 155-130; 163-73; 163-72;

## 2918: TETRAHYDRO MUGUOL

Also called: Tetrahydro-allo-ocimenol (I.F. & F.).

The title name covers a commercial product consisting mainly of:
Tetrahydro-myrcenol = *2,6*-Dimethyl-*2*-octanol
and
Tetrahydro linalool = *3,7*-Dimethyl-*3*-octanol
with smaller amounts of
Dihydro-*alpha*-terpineol.

The three components are all listed in this work under the names mentioned (first) above.

Tetrahydromuguol is therefore not further discussed in this work, while the Acetate of this alcohol-mixture is described under its name "Tetrahydro mugyl acetate".

Tetrahydromuguol is made only by I.F. & F., and is not compounded from the above mentioned, single materials.

It finds extensive use as a soap perfume chemical (mixture) and as a base for many types of floral fragrances, Muguet, Lilac, Rose, Lily, etc. It blends excellently with the conventional "rose materials", alifatic aldehydes, Decenol, Amylcinnamic aldehyde, Butylcyclohexanyl acetate, etc. for such purposes.

Prod.: from Allo-ocimene, via "Allo-ocimenol" (which is a mixture of alcohols) followed by hydrogenation.

IFF-material.

## 2919: TETRAHYDRO MUGYL ACETATE

Tetrahydro-allo-ocimenylacetate.
The commercial product consists of a mixture of:
Tetrahydro myrcenyl acetate = *2,6*-Dimethyl-*2*-octanyl acetate
and
Tetrahydro linalyl acetate = *3,7*-Dimethyl-*3*-octanyl acetate, with smaller amounts of Dihydro-*alpha*-terpinyl acetate = "Menthanyl acetate".

Main components:

$C_{12}H_{24}O_2 = 200.32$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Refreshing, citrusy-herbaceous, mildly floral odor of moderate tenacity.

The title material was marketed as a companion to Tetrahydro muguol after the success of the alcohol (mixture). However, the application of the ester is somewhat more limited, the material not quite as versatile, and its cost (about twice the price of Linalyl acetate) prohibits large-volume use of the material in soap perfumes.

As a novel note in Citrus colognes and for Men's fragrances in general, it offers excellent possibilities. It will support Bergamot, Lavender, Lemon, Petitgrain and many other materials, being more stable than the named natural materials. It also blends well with the light floral materials, and with Labdanum-Styrax-Ambre notes in Fougères, Chypres, etc.

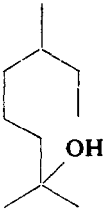
Prod.: by Acetylation of the product called "Tetrahydro muguol" (see monograph).

IFF-1967, samples and commercial material.

## 2920: TETRAHYDROMYRCENOL

*2,6*-Dimethyl-*2*-octanol.

A major component of the commercial product called "Tetrahydro muguol" (see monograph).



$C_{10}H_{22}O = 158.29$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Tetrahydro myrcenol as such is not an important perfume chemical. It forms a major part of the commercially available mixture called "Tetrahydro muguol", in which Tetrahydro linalool is another major component.

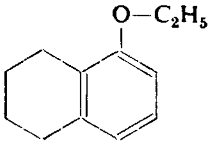
The title material supplies the fresh, citrusy, Lime-like and "lifting" portion of the fragrance picture of "Tetrahydromuguol", while the Tetrahydro linalool supplies the sweet, delicately floral undertones.

The completely hydrogenated (saturated) material or material mixture is more stable towards oxidation or polymerization than the Myrcenol or Dihydromyrcenol, and therefore preferred in soap perfume work. The lack of power in Tetrahydrolinalool is compensated for by the title material, and the total mixture (Tetrahydromuguol) thus represents an attractive and meaningful combination of odor and stability, with the added attraction of low cost in production, since the Tetrahydromuguol mixture is sold as a rectified reaction mixture, not further separated in components.

See also: Dihydro myrcenol (964),
Dihydro-*alpha*-terpineol (970),
*3*-Methylene-*7*-methyl-*1*-octen-*7*-ol (2284),
Tetrahydro linalool (2913),
Tetrahydro muguol (2918).

## 2921: TETRAHYDRO-alpha-NAPHTHOL ETHYLETHER

*1*-Ethoxy tetralin.



$C_{12}H_{16}O = 176.26$

Colorless viscous liquid, solidifying in the cold.

Intensely sweet, tenacious, warm-floral, slightly woody odor.

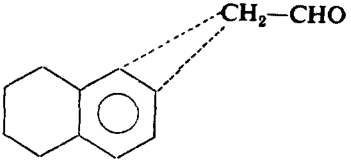
The title material has been suggested for use in perfume compositions, but it does not seem to be commercially available.

Its sweet and pleasant odor may be classified as superior to those of the Nerolins (Naphthol methyl - and ethyl-ethers), but the title material does not have nearly the same power as the Nerolins.

It is reasonable to assume that this material is obsolete, if it ever had any significance at all in perfumery.

31-149;

## **2922:** 5,6,7,8-**TETRAHYDRO**-1-(or-2-) **NAPHTHYLACETALDEHYDE**



$C_{12}H_{14}O = 174.24$

Colorless viscous liquid. B.P. 264° C.

Insoluble in water, soluble in alcohol and oils.

Peculiar, dry-sweet, woody-camphoraceous, relatively tenacious odor with unquestionable Ambregris character.

The title material was quite popular in the years – or generations – before "true" Ambregris chemicals became commercially available. Many derivatives of partially hydrogenated Naphthalene have – at one time or another – been used as Ambregris materials in perfume compositions. A few are still used.

The title material blends very pleasantly with Labdanum products, Styrax, Oakmoss, herbaceous oils (Clary Sage in particular), Galbanum and Vetiver, etc.

It is relatively stable against oxidation and alkali, and it has been used successfully in soap perfumes.

Prod.: from Tetrahydro naphthalene and Carbon monoxide plus Aluminum chloride, plus Ethyl monochloroacetate to yield the glycidate, which is saponified to the title material.

17-34; 5-325; 163-240;

See also:

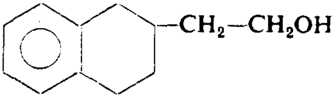
Decahydro-*beta*-naphthaldehyde (823),

Decahydro-*beta*-naphthyl acetaldehyde (825).

## **2923: TETRAHYDRO NAPHTHYL ETHYL ALCOHOL**

Tetrahydro ethyltetralol.

Tetrahydro-*beta-1*-napthyl ethanol.



$C_{12}H_{16}O = 176.26$

Colorless viscous liquid. B.P. over 300° C.

Solidifies in the cold.

Practically insoluble in water, soluble in alcohol and oils.

Camphoraceous-minty, sweet-woody odor of considerable tenacity.

The title material has been suggested for use in perfume compositions as supporting note for herbaceous-woody fragrances, Sage, Rosemary, Lavandin, etc. It blends well with these oils, but does not really contribute attractive character to the composition.

Whenever the material is available at very low cost, it can probably find good use in perfumes for household products, soaps, cleansers, detergents, etc. but it is reasonable to assume that the alcohol is practically obsolete in today's perfumery.

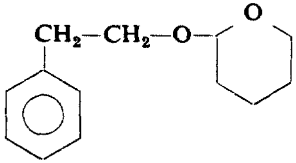
Prod.: from Naphthylmagnesium bromide plus Ethylene oxide by hydrogenation with a Copper chromite catalyst at 200° C. and under high pressure.

68-1326; 68-1343;

## **2924: TETRAHYDRO**-2-**(PHENETHOXY)**-**PYRAN**

Phenylethyl tetrahydro-2-pyranylether.

Tetrahydropyranyl phenylethylether.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and sweet, herbaceous-earthy, rather heavy odor with mildly green notes, and moderate tenacity.

The title ether was developed in search of new Phenylethyl ethers since several of the more conventional ethers had been successful in perfumery, and at least one was found to be a major component of a natural flower oil.

New methods of synthesis of Pyranylethers also encouraged the experiments, and the relationship of the Rose oxides to Tetrahydropyran naturally raised the hopes for the finding of highly interesting derivatives.

The subject ether has found a little use in various floral fragrances, but since the material is not commercially available under its proper chemical name, it has not a very wide distribution.

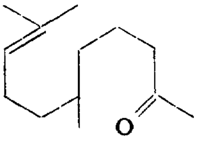
Prod.: from Phenylethyl alcohol and *2,3*-Dihydro-*gamma*-pyran by acid hydrolysis.

See also monographs:
Tetrahydro menthanyl methoxypyran (2915), and Tetrahydro tolyloxy pyran (2929).

69-840; 163-390;

## 2925: TETRAHYDRO-PSEUDOIONONE

*6,10*-Dimethyl-*9*-undecen-*2*-one.
Dihydro geranylacetone.



$C_{13}H_{24}O = 196.34$

Pale straw-colored or almost colorless oily liquid. Sp.Gr. 0.87. B.P. 234° C.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-floral, balsamic odor of rosy-woody character and moderate tenacity.

Pleasant, sweet-fruity, Apple-like or Peach-like taste in concentrations below 20 ppm. Tends to appear bitter-perfumey at higher concentrations.

The title material has been known for many decades, and has been marketed repeatedly under various trade names, usually with very little success.

Occasionally there has been a sudden interest in this ketone, and it does have advantages over Geranyl acetone which tends to oxidize and polymerize. However, contrary to common belief, these materials are far from inexpensive. If their market price can not be brought down to a level, generally acceptable for soap perfumery, there is little chance of these ketones ever becoming standard perfume chemicals for everyday use.

The title ketone finds some use in Rose compositions, where its peculiar oily softness lends very pleasant and natural notes, and also supports mildly green notes in the composition.

It blends furthermore excellently with Vetiver and Labdanum, musks and Lavender products, and it can justly be classified as a very versatile perfume chemical.

The title material is used in small amounts in berry flavors, fruit complexes, etc. at the rate of 1 to 15 ppm in the functional consumer products.

G.R.A.S. F.E.M.A. No.3059.

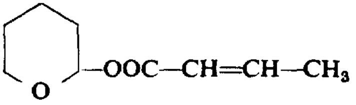
Prod.: Although the material can be made by regulated hydrogenation of Pseudo-ionone, this method may lead to a mixture of Hexahydropseudo-ionone, Tetrahydro-pseudoionone, and possible an isomer of Geranyl acetone.

Other methods use Linalool plus Acetic anhydride with Sodium ethoxide, followed by regulated hydrogenation.

It has also been prepared from Geraniol via Geranyl chloride.

89-367; 163-73;

## 2926: TETRAHYDRO PYRANYL CROTONATE



$C_9H_{14}O_3$ = 170.21

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Warm, soft, oily-herbaceous odor with a floral undertone and moderate to poor tenacity.

This material is rarely offered under its proper chemical name, but it is closely related to Tetrahydrofurfuryl crotonate (an isomer) and more remotely to the Jasmin chemical called "Tepyl acetate", Methylbutyl-tetrahydropyranyl acetate (see monographs).

The title material has found some use in perfume compositions as supporting note in floral bases and specialties.

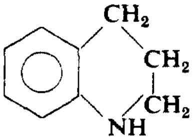
It blends well with Amylcinnamic aldehyde, Rose, Jasmin and Lavender materials, etc. but demands careful fixation or incorporation in a base prior to use in final creations.

Prod.: from *2,3*-Dihydro-*gamma*-pyran plus Crotonic acid by combined acid hydrolysis and esterification.

69-840;

## 2927: TETRAHYDROQUINOLINE

*1,2,3,4*-Tetrahydroquinoline.



$C_9H_{11}N$ = 133.20

Colorless or pale yellowish liquid. It is easily oxidized in air, and may acquire a pale amber color if exposed to air and daylight.

Solidifies in the cold.

M.P. 22° C. B.P. 248° C. Sp.Gr. 1.06.

Slightly soluble in water, soluble in alcohol and oils.

Rather rough or harsh-caramellic-Honey-like, sweet odor with discrete animal character. Not as pronounced animal as Tetrahydro-*para*-methylquinoline.

The material resembles *para*-Methylquinoline with respect to odor, but it has not become nearly as well known or popular in perfumery.

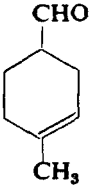
This quinoline is rarely offered commercially, and it could be because of the mentioned lack of "softness" in its initial odor. It is also less versatile than *para*-Methylquinoline, and it is quite possible that the title material could become obsolete in perfumery within the near future.

Prod.: by reduction of Quinoline with Tin and Hydrochloric acid, or with Hydrogen in presence of a catalyst.

31-191; 37-939; 69-642; 156-321;

## 2928: TETRAHYDRO-para-TOLYLALDEHYDE

*4*-Methyl-*3*-cyclohexenealdehyde.
*4*-Methyl-*1,2,5,6*-tetrahydrobenzaldehyde.



$C_8H_{12}O$ = 124.18

Colorless oily liquid. B.P. 169° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, green-leafy odor, very diffusive and of poor tenacity.

The title aldehyde was developed in a program utilizing a new (at that time) method of synthesis for Cyclohexene aldehydes and their alkylsubstituted relatives.

It has found a little use in perfume compositions, mainly in specialties for topnotes, and in bases, often accompanied by alifatic aldehydes, etc. and Citrus oils.

It has a sweeter character than the unsaturated C-6-aldehydes, but is not nearly as powerful or natural as those. As a supporting note in aldehydic bases, however, it has good effect, but it has not yet been offered commercially under its proper chemical name.

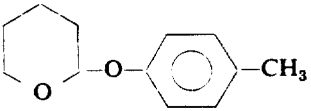
Prod.: from Crotonaldehyde plus Butadiene.

Also from Methylbutadiene and Acrolein.

67-190; 163-363;
See also monograph: Dimethyl butadiene acrolein (966).
(Sample: Dow Chem. Co. 1953).

## 2929: TETRAHYDRO-2-(para-TOLYLOXY)-PYRAN

Tetrahydropyranyl-*2*-tolylether.
Tetrahydropyran-*2*-*para*-cresylether.
*para*-Cresol tetrahydro-*2*-pyranylether.



$C_{12}H_{16}O_2 = 192.26$

Colorless oily liquid. Acquires yellowish or amber-like color when exposed to air.

Almost insoluble in water, soluble in alcohol and water.

Delicately herbaceous, sweet-green odor, reminiscent of fresh wood-sap or fresh, wet bark. Poor storage may cause a slight deterioation, resulting in a perceptible cresylic note in the odor.

The title material is one of many Pyranylethers developed in search of new and interesting series of perfume materials. The green and woody materials are not among the most needed or versatile, but this ether has a record of good performance, in many heavy floral bases, including Jasmin, Tuberose, Gardenia, Narcisse, etc.

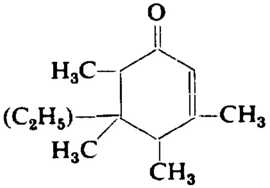
It performs well with Oakmoss and Galbanum in Chypre-types, and with Vetiver and Methylionones, Amylsalicylate, etc.

Prod.: from *2,3*-Dihydro-*gamma*-pyran and *para*-Cresol under conditions of acid hydrolysis.

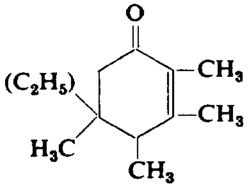
See also: 69-840;

## 2930: TETRAMETHYL ETHYL CYCLOHEXENONE

The commercial material is a mixture of at least two isomers:
*5*-Ethyl-*3,4,5,6*-tetramethyl-*2*-cyclohexen-*1*-one (about 70%) – and
*5*-Ethyl-*2,3,4,5*-tetramethyl-*2*-cyclohexen-*1*-one (about 30%).



Main component.



Minor component.

$C_{12}H_{20}O = 180.29$

Almost colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Warm, caramellic-fruity, slightly spicy or Nut-like odor of considerable tenacity.

The taste is pleasant, creamy-caramellic-fruity at concentrations lower than 40 ppm. Tends to appear "sharp" or "chemical" at concentrations higher than 50 ppm.

The title material (mixture) is used in flavor compositions for imitation Butter, Caramel, various fruit complexes, Rum, and certain berry types. Concentrations vary from 5 to 30 ppm in the finished products.

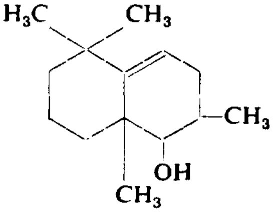
F.E.M.A. No.3061.

The material is cleared for use as a synthetic food flavor in the U.S.A.

See also monographs:
*5*-Methyl-*2*-*iso*-propyl-*1*-acetyl-*5*-cyclohexene (2212),
*1*-Methyl-*4*-propyl-*1*-cyclohexen-*5*-one (2214),
*3*-Methyl-*5*-propyl-*2*-cyclohexenone (2215).

## **2931:** 2,5,5,9-**TETRAMETHYL**-1-**HYDROXY**-1,2,3,5,6,7,8,9-**OCTAHYDRONAPHTHALIN**

*2,5,5,9*-Tetramethyl-*1,2,3,5,6,7,8,9*-octahydro-*alpha*-naphthol.
Tetramethyl octalol.



$C_{14}H_{24}O = 208.34$

White crystalline or opaque mass or granular crystals. M.P. 80° C.

Practically insoluble in water, soluble in alcohol and oils.

Musty-woody-camphoraceous, semi-sweet odor of considerable tenacity. The similarity to Ambregris is more apparent in composition use than in the material as such.

The title secondary alcohol has been suggested for use in perfume compositions as part of Ambregris bases and similar odor complexes.

The material is briefly mentioned in this work as an example of another type of chemicals of Ambregris odor of possible interest to perfumery. It is not offered commercially under its proper chemical name, but it has – to the author's knowledge – not been kept as a secret to the perfume industry, and not been used in captive bases or the like.

The Trimethyl hydroxy-octahydronaphthalin is also known. It has a more animal-Ambre-like note and is not commonly available.

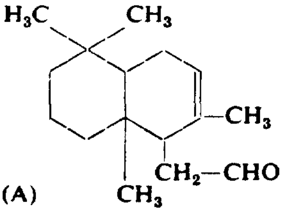
163-380; 163-381; Hoffmann-laRoche patent 1958.

## **2932:** $\Delta^{2,3}$-2,5,5,9-**TETRAMETHYLOCTALYL**-1-**ETHANAL. (A)**

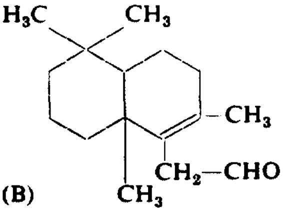
Tetramethyl octahydro-*alpha*-naphthylacetaldehyde.

This monograph includes the isomer:

### $\Delta^{1,2}$-2,5,5,9-**TETRAMETHYLOCTALYL**-1-**ETHANAL. (B)**



(A)



(B)

$C_{16}H_{26}O = 234.38$

Colorless, slightly viscous liquid.
Sp.Gr. 0.99.

Practically insoluble in water, soluble in alcohol and oils.

Musty, mildly woody, and in dilution Ambregris-like odor of good tenacity.

The title aldehydes and the corresponding alcohols (see next) have been suggested for use in perfume compositions.

These materials are not offered commercially under their proper chemical names (perfumers would probably prefer an abbreviated name for easier memorizing), but they have been employed in Ambregris bases of the less expensive type.

It is interesting to notice the similarity in structure between these materials and Squalene (or Ambrein, Sclareol, etc.). The Decalin structure and the Methyl groupings are often repeated features in materials of Ambregris odor.

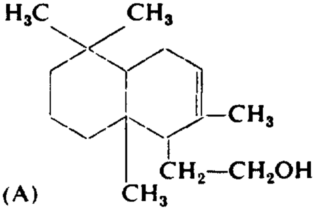
163-380;
U.S. patent No. 2,809,996 (15th Nov. 1957).

## 2933: $\Delta^{2,3}$-2,5,5,9-TETRAMETHYLOCTALYL-1-ETHANOL (A)

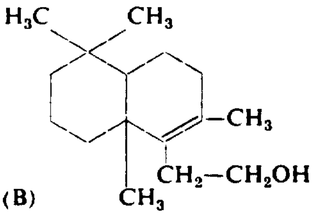
Tetramethyl octahydro-*alpha*-naphthylethylalcohol.

This monograph includes the isomer:

### $\Delta^{1,2}$-2,5,5,9-TETRAMETHYLOCTALYL-1-ETHANOL (B)



(A)



(B)

$C_{16}H_{28}O = 236.40$

Colorless, slightly viscous liquid.

Almost insoluble in water, soluble in alcohol and oils.

Semi-sweet, woody Ambregris-like odor of good tenacity. Less musty but also less powerful than the aldehyde (see previous monograph) and overall sweeter.

These alcohols have been suggested for use in perfume compositions, or in special bases of Ambregris type. The materials are not offered commercially under the proper chemical names.

In view of the development of more true-to-Nature and reasonably priced Ambregris chemicals during the past decade, it is conceivable that materials of the above type may become obsolete.

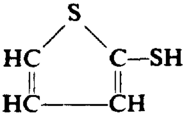
The perfumer is indeed short of truly low-cost materials of pleasant and reasonably natural Ambregris odor type, but the above materials have not been offered and can apparently not be produced at such an attractive cost.

See also comments under the aldehydes (preceding monograph).

163-380;
U.S. pat. No. 2,809,996 (Firmenich, Nov. 15, 1957).

## 2934: 2-THIENYL MERCAPTAN

2-Thienyl thiol.
2-Mercapto thiophene.



$C_4H_4S_2 = 116.21$

Colorless or pale yellowish, mobile liquid. B.P. 166° C.

Very slightly soluble in water, soluble in alcohol and oils.

Very powerful, diffusive and penetrating burnt-caramellic-sulfuraceous odor. It has been claimed that highly purified material has only very faintly perceptible sulfuraceous or "Garlic-like" notes, while the burnt-caramellic notes predominate.

The taste of this material follows the odor – but it is only pleasant at concentrations well below 1 ppm.

Recent literature (Gianturco & Giammarino) report the presence of Thiophene in the volatile portion of roasted Coffee, while the title sulfur derivative is not mentioned. However, the major use of the material is that of a trace component in imitation or "reconstitution" Coffee flavor. Concentrations are kept at about 0.1 ppm in the finished product.

F.E.M.A. No.3062 – cleared for use as a synthetic flavor ingredient by the American F.D.A.

Prod.:

1) by reduction of Thiophen-2-sulfonyl chloride.
2) In the process of making Thiophene from Sodium succinate plus Phosphorus "trisulfide" by heating, the title material becomes a by-product.

69-216; 157-442; 162-739;

## 2935: THIOGLYCOLLIC ACID

Thioglycolic acid.
Mercaptoacetic acid.

$HS—CH_2—COOH$

$C_2H_4O_2S = 92.12$

Colorless liquid. Sp.Gr. 1.33. B.P. 212° C.

Miscible with water, alcohol and oils.

Oxidizes easily in air and produces a disulfide of repulsive odor.

The odor of absolutely pure Thioglycollic acid is mildly sour with a "heavy" or slightly nauseating pungency and poor tenacity.

Commercial grades may show variable amounts of "sulfide" or Hydrogen sulfide off-odor. There are, however, commercial grades of practically no such off odor.

The title material is briefly mentioned in this work although it is probably not used as such in perfumes or flavors. Its name comes up frequently in perfumery literature, because the acid and its salts are used in cosmetic preparations, and – if the acid is not of impeccable olfactory quality – it creates a serious perfumery problem – including a chemical reaction problem. The acid releases Hydrogen sulfide upon decomposition.

Ammonium and Sodium salts of the acid are used in cold-wave preparations. Calcium salt is used as active ingredient in depilatories.

The Baryum salt has been suggested since it is a complex of greater stability, $(S—CH_2—COO)Ba, 3\ H_2O$.

The Mono-ethanolamin- and the Morpholin-salts are also used.

All these are used in alkaline solution, while certain esters of Thioglycollic acid can be used in the so-called "acid cold wave".

Thioglycollic acid discolors in the presence of iron.

Certain esters have been suggested for use in perfumery, and a number of these esters are mentioned in this work.

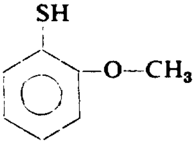
Prod.:

1) from Sodium sulfhydrate plus Sodium monochloro acetate.
2) from Sodium sulfide plus Sodium monochloro acetate to yield Dithioglycollic acid. Electrolysis of the latter acid yields the title material.

66-807; 100-1037; 155-362; B-III-245;

## 2936: THIOGUAIACOL

*2*-Methoxy thiophenol.
*ortho*-Methoxy phenylmercaptan.



$C_7H_8OS = 140.21$

Colorless or pale yellowish liquid.
B.P. 220° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and penetrating, in the undiluted form very unpleasant and sulfuraceous odor. In extreme dilution of quite pleasant, burnt-smokey, warm-caramellic odor of moderate tenacity.

The title material has been suggested for use in imitation Coffee flavor. It has also been suggested for use as a trace component in novel topnote creations for perfumes.

Guaiacol, *4*-Ethylguaiacol and *4*-Vinylguaiacol have all been identified in the volatile portion of roasted Coffee (Gianturco, 157-443), but the title material has not been mentioned as a known component.

Many mercaptans and other sulfur derivatives of such known Coffee flavor component have been experimentally tested in Coffee imitation flavor, some with good results.

The title material is not listed as G.R.A.S. in the U.S.A.

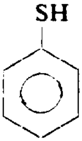
Prod.:

1) from *ortho*-Aminophenol-methylether via Diazoreaction.
2) from Sodium phenoxide plus Sulfur at 200° C. to yield *2:2'*-Dihydroxy-diphenyl-disulfide. Reduction and Methylation afford the title ether.

68-470; 157-443;

## 2937: THIOPHENOL

Benzene thiol.
Phenyl mercaptan.



$C_6H_6S = 110.17$

Colorless or pale yellowish mobile liquid.
B.P. 169° C. Sp.Gr. 1.08.

Insoluble in water, soluble in alcohol and oils.

Highly purified material has a very powerful, but initially not sulfuraceous or "garlic-like" odor, yet this Garlic-note will appear eventually when the material is exposed to air. It is therefore difficult to define the actual odor of the material in the state of functional use.

Commercial grade material normally shows Garlic-like, diffusive rubber-like odor, according to the degree of dilution.

The taste is rather sweet, nondescript at concentrations below 5 ppm.

The title material is very unstable under alkaline conditions, in presence of metals, oxidizing of reducing agents, Olefins, Ketones, Aldehydes, air, etc.

One of the oxidation products is Diphenyl disulfide, which has a pronounced Garlic-like odor.

The title material has found some use in flavor compositions as a trace ingredient in imitation Coffee flavor.

It is approved for use as a synthetic flavor chemical by the American F.D.A.

Prod.: by reduction of Benzene sulfonylchloride with nascent Hydrogen.

68-433; 100-1040; 159-511; 162-739;

## 2938: THIOPROPANAL-S-OXIDE

Propyl thioaldehyde sulfoxide.
"Onion lachrymator".

$CH_3-CH_2-CH=S=O$

$C_3H_6OS = 90.15$

The title material has been suspected of being the lachrymator of Onions. It is an extremely unstable chemical, and although this is in accordance with the common experience that the lachrymatory effect of Onions is of short duration and only appears when Onions are bruised or comminuted, there is still doubt about the identity of the true lachrymator (or lachrymators) in Onion.

Recent investigations have pointed in the direction of a related chemical:

*1*-PROPENE SULFENIC ACID

$CH_3-CH=CH-S-OH$

which is an empirical isomer of the above sulfoxide.

$C_3H_6OS = 90.15$

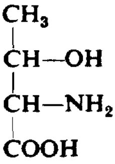
It remains to be confirmed exactly which material is responsible for the lachrymatory effect, although this has long since been proven to have no significant importance to the flavor of Onions. The above materials would both be completely destroyed in cooking, frying, boiling, broiling, etc. and the Onion is mainly consumed in a state of non-lachrymatory, but highly aromatic vegetable product.

The above material(s) are included in this work since the author believes that they are of potential interest and will have increasing importance in the future study of food flavor components.

66-354; 68-244; 69-381; 158-144; 157-398;

## 2939: THREONINE

*alpha*-Amino-*beta*-hydroxybutyric acid.
*2*-Amino-*3*-hydroxybutanoic acid.
(The *L*- and *DL*-forms are used).
(The data below refer to *L*-Threonine).



$$\begin{array}{l} CH_3 \\ | \\ CH-OH \\ | \\ CH-NH_2 \\ | \\ COOH \end{array}$$

$C_4H_9NO_3 = 119.12$

White crystals or powder. Decomposes near melting point at 257° C.

Soluble in water, Insoluble in absolute alcohol and oils.

Practically odorless when pure, but may carry faint odor depending upon method of production.

Mild and sweet, nondescript taste in concentrations near 1000 ppm.

Although the subject Aminoacid is not classified as a perfume or flavor material, it is briefly mentioned here because of its extensive use as a dietary nutrient with a mildly sweet taste. It has also been used occasionally as part of Maple flavor complexes.

The title acid, its hydrochloride salt, its hydrate or anhydrous form, are all classified as G.R.A.S. (as nutrient) in the U.S.A.

Prod.:

1) by isolation from natural Proteins.
2) synthetic (many methods) e. g.: from Ethyl acetoacetate by Nitrosation, followed by reduction, treatment with Thionylchloride and finally hydrolysis.

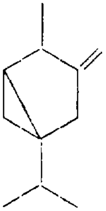
58-III-54; 60-V-59; 66-1070; 100-1043; 162-739;

See also: Aminobutyric acid (110), – and Serine (2844).

## 2940: THUJONE

Tanacetone (this synonym actually refers to *beta*-Thujone from Tanacetum oil).

The general description below refers to *alpha*-Thujone, sometimes called *laevo*-Thujone, which is the most commonly occurring of the two isomerides.



$C_{10}H_{16}O = 152.24$

Almost colorless mobile liquid. Sp.Gr. 0.92. B.P. 201° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and penetrating, warm-herbaceous, minty-camphoraceous odor of moderate to poor tenacity.

The material tends to darken and resinify upon exposure to air.

Warm-herbaceous, bitter taste in concentrations lower than 10 ppm. Higher concentrations produce pungent-bitter, herbaceous taste.

The title monoterpenoid ketone is used sparingly in certain perfume formulations, often as a trace component of topnote compositions, and it blends very well with Oakmoss, Rosemary, Geranium, Galbanum and various green-herbaceous notes, and with certain Ambre-type fragrances.

It is common practise to use natural oils, containing Thujone for similar effects, or more attractive effects.

Thujone has been in the limelight for its physiological effects, not fully elucidated, and poorly included in perfumery literature, for many decades. Herbs, containing essential oils in which Thujone forms a major component, have been under suspicion by the food authorities, and many products containing Thujone-bearing oils or extracts, have been banned from food, beverages, etc.

The toxicity of Thujone is roughly estimated at three times that of Nitrobenzene, but it is not possible to compare the two, since the effect of Thujone is entirely different, sometimes classified as "Curare-like" or paralyzing on the human CNS or heart system. The Thujone content of certain Artemisia species, used in "Absinth" alcoholic beverage, was responsible for the ban of certain brands of alcoholic beverage in the 1930's in France.

Thujone is by some authorities considered the most toxic of all commonly occurring components of essential oils.

Prod.: by isolation from various essential oils: Cedarleaf oil (Thuja oil), Tansy oil, Dalmatian Sage oil, etc.

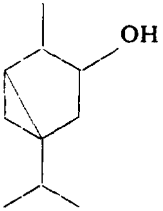
The synthesis from Thujaketonic acid has no commercial interest as long as the above oils are freely available.

67-549; 67-552; 85-113; 89-270; 89-278; 100-1044; 163-73; 163-241; B-VII-93;

## 2941: THUJYL ALCOHOL

Tanacetyl alcohol.

The commercial product is a mixture of stereoisomerides, according to the Nature of the starting material, and to the conditions of isolation from the natural oil.



$C_{10}H_{18}O = 154.25$

The most desirable isomer (by general opinion) is the *laevo*-Thujylalcohol, which is a solid, crystalline material. M.P. 67° C.
B.P. 206° C. Sp.Gr. 0.93.

It has a powerful, minty-camphoraceous, Lime-like character of odor and moderate tenacity.

The second-most desirable isomer is the *dextro-iso*-Thujylalcohol which is an oily liquid of pleasant, sweet-herbaceous, citrusy odor.

The least desirable isomer, *laevo-neo*-Thujylalcohol is crystalline, but melts at 23° C. It has a bitter-camphoraceous odor.

Since Thujone-bearing oils are relatively common and available, the derivatives of Thujone have been known for a long time. However, it was not until the perfume industry was seriously searching for chemicals with Lime-type odor (and preferably of oxygenated type), that the title material became interesting.

Thujyl alcohol is stable in soap and other consumer products, and it blends well with the herbaceous oils, Citrus oils, etc. for refreshing odor types in household products, room sprays, etc.

There is no complete agreement about the type of odor preferred in Thujyl alcohol, and the few manufacturers of the material offer Thujylalcohols of widely different odor characteristics. Most of the products are mixtures of several stereoisomerides, but the trend seems to point in favor of the above named preferred and second-most preferred isomers.

The pure isomers are rarely offered commercially.

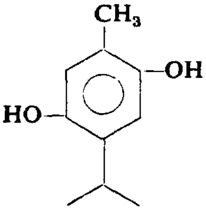
Prod.: by reduction of Thujone with Sodium and alcohol. The yield is a mixture of isomers, resembling the Menthol mixture from Menthone. The title material has also been prepared from Sabinol by catalytic hydrogenation or by reduction with Sodium in alcohol.

Thujyl alcohol is considered much less toxic than Thujone, but the alcohol is – to the author's knowledge – not used in flavors.

67-549; 85-114; 88-136; 1-707; 95-101; 96-84;

## 2942: THYMOHYDROQUINONE

*2*-Methyl-*5*-*iso*-propylquinol.
*2*-Methyl-*5*-*iso*-propylhydroquinone.
Hydro-thymoquinone.



$C_{10}H_{14}O_2 = 166.22$

Prismatic crystals. M.P. 142° C.
B.P. 290° C. Sublimes when heated.

Slightly soluble in cold water. Soluble in hot water and alcohol. Practically insoluble in oils.

Dry-woody, herbaceous-spicy odor of considerable tenacity. The herbaceous-spicy notes resemble Anise and Fennel, but do not have the palatable sweetness or attractive aroma of these oils.

The taste is equally woody-herbaceous, spicy, woody-Fennel-like at concentrations near 20 ppm. Bitter at higher concentrations.

The title phenol has been suggested for use in perfume compositions, and years ago also in flavors.

Since Fennel oil has very little application in perfumes, and only high-grade Fennel oil has interest to the perfumer at all, the need for such chemical is very limited.

The Methylether (see next) has more to offer, and has had some application in perfumery.

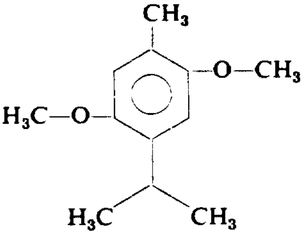
The title material can be considered as practically obsolete in perfumery.

Prod.: by reduction of Thymoquinone with Sulfurous acid or with the aid of a catalyst.

68-478; 90-414; 95-119; 96-98; 163-241; B-VI-945;

## 2943: THYMOHYDROQUINONE DIMETHYLETHER

*2*-Methyl-*1,4*-dimethoxy-*5*-*iso*-propylbenzene.
*2,5*-Dimethoxy-*para*-cymene.



$C_{12}H_{18}O_2 = 194.28$

Colorless or pale straw-colored, oily liquid. B.P. 250° C. Sp.Gr. 0.99.

Practically insoluble in water, soluble in alcohol and most oils.

Heavy-sweet, warm-spicy, almost nut-like earthy odor of considerable tenacity. The resemblance to Fennel is not very apparent in the undiluted material, but becomes more conspicuous in compositions or in dilution. Various trade names using the word "Fennel" as part of the name may lead a customer to believe that the title chemical is a key to Fennel odor.

The subject ether is, in fact, chief component of the essential oil of "Dog Fennel" growing wild in the Southeastern United States, but not commercially exploited. The plant is not related to true Fennel, but it is closely related to the Liatris plant, used in Tobacco flavoring.

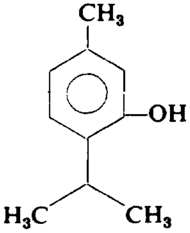
The ether has been suggested for use in perfume compositions as a fixative with considerable sweetening effect, or as a modifier for Coumarin in novel Fougère types, Chypres, etc. It blends well with Lavender, Oakmoss, Amylsalicylate, etc. for such purposes.

Prod.: by Methylation of Thymohydroquinone (see monograph) in aqueous alkaline solution with Dimethylsulfate.

68-478; 90-477; 95-120; 96-98;

## 2944: THYMOL

*1*-Methyl-*3*-hydroxy-*4*-*iso*-propylbenzene.
*para*-*iso*-Propyl-*meta*-cresol.
*3*-*para*-Cymenol.
*alpha*-Cymophenol.
*alpha*-Oxycymol.
*5*-Methyl-*2*-*iso*-propylphenol.
*3*-Methyl-*6*-*iso*-propylphenol.
"Thyme camphor".
*3*-Hydroxy-*para*-cymene.
*meta*-Thymol.



$C_{10}H_{14}O = 150.22$

Translucent crystals. M.P. 51° C.
B.P. 233° C. Sp.Gr. 0.95 (liquid), but the crystals sink in water at 20° C.

0.1% soluble in water, soluble in alcohol and oils. The material forms liquid mixtures with Camphor, Menthol, Quinine sulfate and many other solids.

Powerful, sweet-medicinal, herbaceous and warm odor of moderate tenacity. The odor is much more pleasant than that of Phenol (or Cresol) and not nearly as "dry-tarry" as that of Carvacrol (isomer of Thymol).

The taste is pleasantly sweet-medicinal, herbaceous-spicy at concentrations up to 20 ppm (Thymol alone) or much higher in compositions (100 ppm in the presence of Menthol-Eucalyptol etc. is still not unpleasantly medicinal).

Thymol is strongly antisceptic, but relatively non-toxic. It is estimated that Thymol is about 5 times less toxic than Phenol by human ingestion. Thymol has been known and isolated since 1853.

It is used in discrete amounts in perfumes, although Thyme oil is often preferred for its mellower, softer effect and its reasonable cost. Inexpensive synthetic Thymol has appeared on the world market since 1960 when the price fell considerably below that of Menthol.

Thymol is more commonly used in flavor compositions, mainly in toothpaste flavor, cough drops, mouth washes, gargles and chewing gums. It is often used partly for its antiseptic effect in such products. The concentration may vary from 2 to 100 ppm, highest in chewing gums.

A newer use of Thymol is that in imitation Mandarin flavor, since the material was identified in Mandarin peel oil in 1963. It blends excellently with Citrus, Mint, Spice and herbaceous flavor materials or with fruity complexes.

F.E.M.A. No.3066. G.R.A.S.

Prod.:

1) from *para*-Cymene or from Nitrocuminaldehyde.
2) from *para*-Cresol via its Sulfonate to the *iso*-Propyl-derivative.
3) from Piperitone by dehydrogenation. The process yields Menthol plus Thymol. The two materials can be satisfactorily separated.
4) The process of isolation from Ajowan oil is only of local importance.

1-437; 5-281; 31-24; 31-34; 68-421; 85-115; 90-401; 95-116; 96-98; 100-1045; 104-51; 104-616; 106-338; 159-624; B-VI-532;

## 2945: iso-THYMOL

"Antioxine".

See monographs on Carvacrol and Thymol.

The title material is not used as such in perfumes or flavors, but has has found some use as a preservative in cosmetic preparations. Due to its pronounced (medicinal) odor, it has practically been abandoned in favor of newer and less odorous bactericides or fungicides.

However, since there are seven (7) commercially available isomers with the Thymol type structure, the author finds it of possible interest to briefly list these materials, most of which are of no use to the perfumer or flavorist:

1) *5*-Methyl-*2*-*iso*-propylphenol = Thymol (solid).
2) *6*-Methyl-*3*-*iso*-propylphenol = Carvacrol (liquid).
3) *2*-Methyl-*6*-*iso*-propylphenol, a liquid.
4) *2*-Methyl-*4*-*iso*-propylphenol, a liquid.
5) *3*-Methyl-*5*-*iso*-propylphenol, a solid.
6) *3*-Methyl-*2*-*iso*-propylphenol, a solid.
7) *3*-Methyl-*4*-*iso*-propylphenol, a solid.

The cosmetic literature refers to *iso*-Thymol as a liquid, and there are only two candidates for that description, Nos. 3) and 4) with boiling points respectively 226° C. and 231° C. Theoretically, Carvacrol is also a liquid isomer of Thymol, but the odor of the commercial *iso*-Thymol does not at all resemble that of Carvacrol. It is weaker, less tarry, more typical "phenolic"-medicinal.

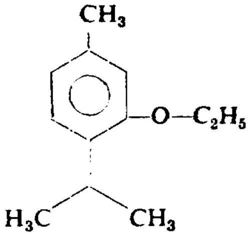
When Thymol is manufactured from *para*-Cresol, a by-product is obtained and it is named *iso*-Thymol. It consists of a mixture of *ortho*-, *meta*- and *para*-Thymols. The highest melting point has item No. 7 (114° C.) but the isomer mixture is liquid. Most conceivably, the isomer mixture has been offered as such – an ill-defined mixture of isomers, poor in Thymol and Carvacrol, mainly consisting of items No. 3-4-5-6-7.

The author is of the impression that the title material is almost obsolete as a cosmetic preservative.

68-422; 90-406; 155-357;

## 2946: THYMOL ETHYLETHER

*1*-Methyl-*3*-ethoxy-*4*-*iso*-propylbenzene.
*3*-Ethoxy-*para*-cymene.
*para*-*iso*-Propyl-*meta*-cresol ethylether.



$C_{12}H_{18}O = 178.28$

Colorless oily liquid.
B.P. 228° C. Sp.Gr. 0.92.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, earthy-rooty, mildly spicy odor of moderate tenacity. Odor descriptions often include the word "Thymol-like", but the author finds that a high-quality ether has no resemblance to Thymol in its odor, except the warm-spicy character.

The title ether has been suggested for use in perfume compositions as a modifier in mildly spicy fragrance types, with Coumarin, Methyleugenol, Amylsalicylate, Labdanum, etc. for Fougères, etc.

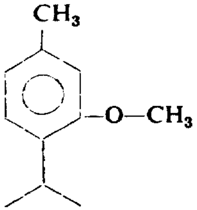
The material is very rarely offered commercially, and the author is of the impression that it is almost obsolete in perfumery.

Prod.: from Thymol in weak aqueous alkaline solution with Diethyl sulfate.

31-142;

## 2947: THYMOL METHYLETHER

*1*-Methyl-*3*-methoxy-*4*-*iso*-propylbenzene.
*3*-Methoxy-*para*-cymene.



$C_{11}H_{16}O = 164.25$

Colorless oily liquid.
B.P. 216° C. Sp.Gr. 0.93.

Practically insoluble in water, soluble in alcohol and oils.

Warm-spicy-rooty, herbaceous odor with practically no trace of medicinal or "phenolic" notes, but rather a dry-leafy character. Moderate tenacity.

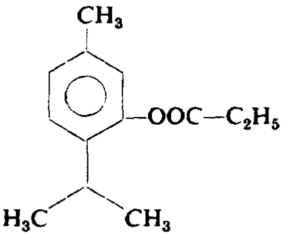
The odor of this material is rather pleasant, but lacks character, and the type of odor is not frequently wanted in perfumery. It may serve as a modifier in mildly spicy fragrances, as a companion to Methyleugenol for "Tea-like" notes, in Chypre or Fougère variations, in detergent fragrances, etc.

Prod.: from Thymol in weak aqueous alkali with Dimethylsulfate.

90-463; 95-117; 163-73;

# 2948: THYMYL PROPIONATE

*3*-Methyl-*6*-*iso*-propyl phenylpropionate.



$C_{13}H_{18}O_2 = 206.29$

Colorless oily liquid. B.P. 260° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, warm-spicy, herbaceous odor of good tenacity. The odor has little similarity to that of Thymol, being absolutely "non-medicinal" and much milder than that of Thymol.

The title material was developed by one of the manufacturers of synthetic Thymol in the U.S.A. It has remained a curiosity on the perfumer's shelf ever since, and very little interest has been shown in the ester. In view of the relatively low odor value of the title material and its cost well above the "large-volume" soap/detergent fragrance chemicals, it is most conceivable that the ester will slowly become obsolete in perfumery.

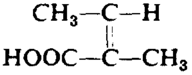
If the cost would be equal to that of the commonly used soap perfume chemicals, it could undoubtedly find use in new "fresh" fragrances as variations from the conventional types. It blends well with Lavandin, Rosemary, Terpineol, Amylsalicylate, etc. for such purpose.

Prod.: from Thymol and Propionic anhydride.

Sample: Newport Industries – Tenneco Inc., U.S.A.

# 2949: TIGLIC ACID

*trans*-*2*-Methyl-*2*-butenoic acid.
*trans*-*2*-Methylcrotonic acid.
*trans*-*alpha*-*beta*-Dimethylacrylic acid.
*trans*-*alpha*-Methylcrotonic acid.



$$\begin{array}{l} CH_3{-}C{-}H \\ \qquad\ \ \| \\ HOOC{-}C{-}CH_3 \end{array}$$

$C_5H_8O_2 = 100.12$

Perfume chemistry literature is not in complete agreement about the *cis*-*trans*-configuration of Tiglic and Angelic acids. The author has used the *trans*-configuration for Tiglic acid, based upon a majority of recent information speaking in favor of Angelic acid being the unstable *cis*-form, while Tiglic acid is the more stable *trans*-form.

M.P. 64° C. B.P. 199° C.

Slightly soluble in water, soluble in alcohol and oils.

Spicy-rooty, sweet-sour herbaceous odor of moderate tenacity.

Spicy-warm, slightly sour taste in concentrations near 50 ppm. The acidulous taste fades away at lower concentrations, leaving only the pleasant, spicy-rooty taste.

The undiluted acid is an irritant, and its vapors have a vesicant effect upon human skin.

In spite of the fact that the acid is a naturally occurring component of many essential oils, extracts and spice oleoresins, it has not been approved for use as a food flavor in the U.S.A.

It finds limited use in perfume compositions, mainly as a trace ingredient in artificial essential oils.

Many esters of Tiglic acid are used in perfumes and artificial essential oils.

Prod.:

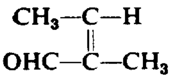
1) from *2*-Hydroxy-*2*-methylbutyronitrile.
2) by condensation of Methylmalonic acid with Paraldehyde in presence of Acetic acid plus Acetic anhydride.

Hydrogenation of Tiglic acid yields *2*-Methylbutyric acid, which has found considerable use in the form of esters in perfumes and flavors.

66-636; 100-1047; 90-119; 140-144; B-II-430; 1-209; 104-158;

## 2950: TIGLIC ALDEHYDE

*alpha*-Methyl crotonaldehyde.
*trans*-Dimethyl acrylic aldehyde.



$$\begin{array}{l} CH_3\text{—}C\text{—}H \\ \qquad \| \\ OHC\text{—}C\text{—}CH_3 \end{array}$$

$C_5H_8O = 84.12$

Colorless mobile liquid.
Sp.Gr. 0.87. B.P. 118° C.

2.5% soluble in water, miscible with alcohol and oils.

Easily oxidized in air.

Very diffusive, penetrating odor, unpleasantly pungent, irritating when undiluted, but quite pleasant, fruity-herbaceous in extreme dilution. Very poor tenacity.

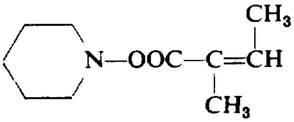
The title aldehyde has found a little use in perfume compositions mainly as a trace component in special topnote compositions, bases, etc. It will support fruity, green and vinous notes, and it has interesting effects in Geranium, Clary Sage, etc.

Prod.: by condensation of Acetaldehyde with Propionaldehyde.

66-503; 1-169; B-I-733;

## 2951: TIGLYL PIPERIDIDE

Piperidine tiglate.
Pentenoyl piperidide.
*trans-2*-Methyl butenoyl piperidide.



$C_{10}H_{17}NO_2 = 183.25$

Almost colorless, oily liquid, solidifying in the cold.

Slightly soluble in water, soluble in alcohol and most oils.

Mild, but in high concentration nauseating, sweet-herbaceous, almost tobacco-like odor, in dilution very pleasant, warm and herbaceous, of good tenacity.

The taste is pungent, with slightly delayed pungency, and not nearly as powerful as Piperonyl piperidine or other known Pepper-pungency materials.

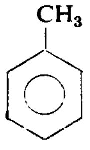
This material has been suggested for use in perfume compositions as part of a herbaceous complex in heavy floral fragrances, Ambres, etc. It has a much more pleasant effect than Piperidine itself, and is less animal in olfactory character.

Prod.: from Piperidine and Tiglyl chloride.

69-572;
See also monographs:
Nonanoyl vanillylamide (2353),
Piperine (2627),
Piperidine (2626).

## 2952: TOLUENE

Toluol.
Methylbenzene.
Phenylmethane.
Methacide.



$C_7H_8 = 92.14$

Colorless mobile liquid.
Sp.Gr. 0.87. B.P. 111° C.

Very slightly soluble in water, miscible with absolute alcohol, soluble in perfume alcohol and in oils.

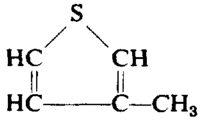
Flammable liquid. The vapors form explosive mixtures with air at room temperature.

The title aromatic hydrocarbon is not a perfume or flavor material, but it is included in this work because it is used as a solvent for extraction of active ingredients in plant materials, etc.

Pure toluene has a sweet-gassy odor, milder than that of Benzene. It is much less toxic than Benzene (estimated 20 to 50 times less toxic to human skin and respiratory system).

For extraction purposes the Toluene should be free from *beta*-Thiotolene, a material similar to Thiophene in crude Benzene:

Thiotolene:



also called *beta*-Methyl thiophene, is a liquid of penetrating and repulsive odor. Its boiling point (115° C.) is so near that of Toluene, that ordinary distillation does not satisfactorily remove the undesirable component. Since it is higher boiling, it is also more perceptible (actually concentrated) in extracts made with Toluene and where the solvent has been incompletely removed.

Toluene is an excellent solvent for resins, sesquiterpenes, etc. and has also been used in the initial extractions of Oakmoss.

Prod.:

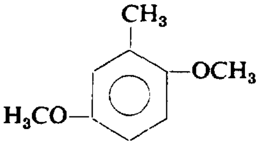
1) by isolation from the "Light Oil" fraction of petroleum tar oil.
2) by cyclodehydrogenation of Heptane (newer method).

1-394; 34-806; 68-106; 100-1052; B-V-280;

## 2953: TOLUHYDROQUINONE DIMETHYLETHER

*2,5*-Dimethoxytoluene.
*2*-Methylhydroquinone dimethylether.

NOTE: Perfumery literature occasionally refers to "Toluquinone dimethylether", which is confusing. Toluquinone is not identical to Toluhydroquinone.



$C_9H_{12}O_2 = 152.20$

White crystalline material.

Almost insoluble in water, fairly soluble in alcohol, soluble in most oils.

Warm, spicy-haylike and very tenacious odor.

The title material, also sometimes confused with Thymohydroquinone dimethylether, which has a related odor, has found a little use in perfume compositions.

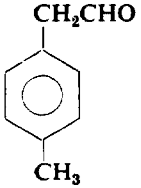
Its odor type is more anisic-fennel-like than Hydroquinone dimethylether, and less nutlike. The material blends very well with the herbaceous oils, Oakmoss, Amylsalicylate, Galbanum, etc. for Chypres, Fougères, Lavender compositions, etc. and it has good effect as a fixative.

Prod.: from *ortho*-Toluquinone by reduction to Toluhydroquinone. The latter is treated with Dimethylsulfate in weak aqueous alkaline solution to produce the title ether.

68-478;

## 2954: para-TOLYL ACETALDEHYDE

*para*-Methyl phenylacetaldehyde.
Ecorsal (name also used for Hydratropaldehyde = 1696).
Sylvanal (name also used for Hydratropaldehyde = 1696).
Syringa aldehyde. (Do not confuse with Syringic aldehyde).
"Vert de Fleurs" (name also used for Hydratropaldehyde = 1696).



$C_9H_{10}O = 134.18$

Colorless oily liquid.
Sp.Gr. 1.00. B.P. 210° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful and refreshing green-fruity, "forest-like", sweet, floral odor of moderate tenacity. The undiluted material has a rather sharp initial odor, but sweetness predominates in the diluted product.

The taste is sweet-fruity, mildly green at concentrations near 10 ppm.

This aldehyde is used in perfume compositions where sweet-green notes are compatible with floral notes- e. g. in Lilac, Hyacinth, Rose, Sweet Pea, etc. and in woody Chypres, New Mown Hay types, "forest odors" etc. It offers a very pleasant variation of the harsher Phenylacetaldehyde, and it is much easier to use, does not "fade" as quickly in the composition, and enhances sweet-fruity notes in an attractive manner.

The material is also used in flavor compositions, mainly in imitation Honey, Banana, Bitter almond, Plum, Gooseberry, Nut, Coconut, etc.

Concentrations in the finished product are usually very low, about 2 ppm.

G.R.A.S. F.E.M.A. No.3071.

Prod.:

1) from *para*-Methylbenzaldehyde via Darzen's reaction.
2) from *para*-Methylbenzylchloride plus Hexamethylene tetramine.

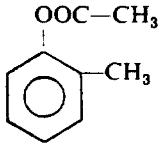
See also monograph: *alpha*-Methyl phenylacetaldehyde (= Hydratropic aldehyde).

155-130; 156-296; 163-52; 163-73; 163-224; 163-363;

## **2955:** ortho-**TOLYL ACETATE**

*ortho*-Cresyl acetate (correct name).
Acetyl-*ortho*-cresol.

NOTE: The title name "Tolyl" has been used because it is commonly applied to this material in perfume and flavor literature.
It should not be confused with "true" *ortho*-Tolyl acetate, which is the acetate of 2-Methyl benzylalcohol (see monograph: *ortho*-Tolyl alcohol). The "true" *ortho*-Tolylacetate is – to the author's knowledge – not used in perfumes or flavors.



$C_9H_{10}O_2 = 150.18$

Colorless liquid. B.P. 208° C.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, fruity-medicinal odor, in dilution sweet, floral and more pleasant. Poor tenacity.

Concentrations below 10 ppm have a sweet-creamy, slightly fruity taste, but higher concentrations – particularly with impure material – produce a medicinal or harsh taste.

Odor- and flavor descriptions of this material are often clearly based upon the study of entirely different material, presumably the "true" Tolyl acetates, which have all pronounced fruity and distinctly sweet taste. The author suspects that confusion could very well have arisen at an earlier stage, so that the Cresyl acetates "accidentally" entered the flavor laboratory, not the Tolyl acetates.

The confusion is not diminished by the fact that both series are used and known to perfumers and flavorists. This is particularly confusing to the suppliers of these materials.

The title material is (allegedly) used in Butter, Caramel, Cherry, Honey flavors and fruit compositions at concentrations from 1 to 10 ppm in the finished product.

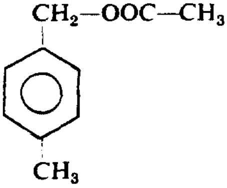
G.R.A.S. F.E.M.A. No.3072.

Prod.: from *ortho*-Cresolsodium and Acetic anhydride.

68-431; 163-358; B-VI-355;

## 2956: para-TOLYLACETATE

*para*-Methyl benzylacetate (correct name).
*4*-Methyl benzylacetate.
The commercial product is mainly the *para*-isomer, occasionally with some *ortho*-isomer. Do not confuse this material with *para*-Cresyl acetate, which is sometimes called *para*-Tolyl acetate.



$C_{10}H_{12}O_2 = 164.21$

Colorless liquid. B.P. 222° C. Sp.Gr. 1.04.

Almost insoluble in water, soluble in alcohol and oils.

Sweet, floral-fruity and mildly green-herbaceous odor of moderate tenacity. Sweeter and less harsh than Benzylacetate, longer lasting and richer.

Sweet-fruity, slightly herbaceous (spicy-warm) taste in concentrations below 40 ppm. Rather pungent at higher levels.

This ester has found increasing use in perfume compositions, although its price is many times that of Benzylacetate. But since the effect of the title material in Jasmin bases and compositions is far superior to that of Benzylacetate, the higher cost causes only little reluctance in using the Tolylester. It blends excellently with Jasmin materials, Hyacinth, New Mown Hay, Gardenia, etc. and gives very good results with the Pyranylether and -ester specialties (Jasmal, Tepylacetate, etc.). A steady increase in the demand and use of this material may also lower the market cost and further help making it a common fragrance chemical for everyday use.

It gives very sweet and pleasant fruity effects in Banana, Cherry, Butter, Caramel, Honey, Nut and Spice flavors, fruit complexes (tutti-frutti for chewing gum, etc.) and is used at concentrations from 1 to 10 ppm in most finished products, except in chewing gum where it may be as high as 200 ppm.

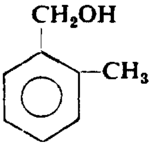
Prod.: from *para*-Tolylalcohol by Acetylation (see *para*-Tolyl alcohol).

The commercial product consisting of mixed isomers, *ortho-*, *meta-* and *para*-Tolylacetate, is classified as a synthetic flavoring substance and approved for food flavor use by the American F.D.A.

163-48; 163-73; 163-219; 163-358; 162-662;
See also 1915.

## 2957: ortho-TOLYL ALCOHOL

*2*-Methylbenzylalcohol.
*ortho*-Methyl benzylalcohol.
*ortho*-Tolylcarbinol.



$C_8H_{10}O = 122.17$

White crystals. M.P. 36° C. B.P. 223° C.

Very slightly soluble in water, soluble in alcohol and oils.

Mild, floral odor, overall rosy, but also musty, sweet and moderately tenacious. The odor is more floral than that of Phenylethyl alcohol, but somewhat weaker.

This material has been suggested for use in perfume compositions, and it is occasionally available, since it can be produced on a commercial scale. It is not nearly as well known as the *para*-isomer, however, and one reason may be that it is difficult to produce in such a state of purity that it remains solid at storage temperature.

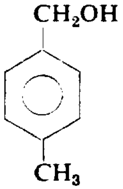
As a base for Rose, Lilac, Appleblossom and other mild florals, and as a modifier in many herbaceous fragrance types, it blends well with the conventional materials, but tends to dull the overall fragrance, in other words, it needs skillful addition of powerful odorants or topnote complexes.

Prod.: from Benzyl magnesiumchloride and Formaldehyde. The method is rather unique for this isomer.

68-497; 68-499; 163-73; 163-358;
See also monograph: *para*-Tolylalcohol.

## 2958: para-TOLYL ALCOHOL

*4*-Methyl benzylalcohol.
*4*-Tolyl carbinol.
*para*-Methylbenzylalcohol.
The commercial product consists mainly of the *para*-isomer. Some products are almost pure *para*-isomer.



$C_8H_{10}O = 122.17$

White crystals, granular or crystalline powder, sometimes fused lumps. M.P. 60° C. (better grades). B.P. 217° C.

Very slightly soluble in water, soluble in alcohol and oils.

Faint, but very pleasant, green-rosy, leafy and sweet-balsamic odor of moderate tenacity.

This material is rarely offered under its proper chemical name, and until a few years ago, it was still absent from the shelves of most perfume laboratories. Improved technique and perhaps new methods of synthesis have made the material commercially available at a more attractive price.

It blends excellently with all the conventional materials, floral and non-floral, and offers good basis for experiments with new variations of Lilac, Rose, Appleblossom, Geranium, Fougère, etc. It is stable in soap and compatible with all the "troublesome" fragrance chemicals. As a companion to high-grade Terpineol in Lilac fragrances, it is one of the most useful low-cost materials.

Prod.: (many methods) e. g.

1) from *para*-Tolyl magnesium bromide plus Acetaldehyde.
2) by hydrolysis of *para*-Methyl benzyl chloride.

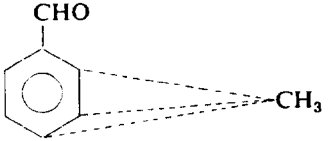
68-127; 68-499; 163-73; 163-219; 163-358;
Sample: Ogawa & Co., Ltd. (Japan).

## 2959: TOLYL ALDEHYDE

"Tolualdehyde".
This monograph describes the commercial product which is a mixture of the *ortho-*, *meta-* and *para*-Tolylaldehydes:

*2*, *3*, *4*—Methylbenzaldehyde.

The individual isomers are also commercially available and will be described separately following this monograph.



$C_8H_8O = 120.15$

Colorless oily liquid. Sp.Gr. 1.03.

Slightly soluble in water, soluble in alcohol and oils.

Sweet-herbaceous, Bitter-almond-like moderately tenacious odor. Not as pungent as Benzaldehyde, but more herbaceous-warm.

Intensely sweet, warm-fruity and Bitter-almond-like taste in concentrations lower than 500 ppm. Pungency increases at this level, while the pleasant and perceptible flavor reaches below 10 ppm.

The title aldehyde finds some use in perfume compositions, mainly of the Lilac and New-Mown-Hay type, also Sweet Pea, Ylang etc. The *para*-isomer is generally preferred for perfumery work, but since the mixed isomers consists of predominantly the *para*-isomer, there is some economic advantage in using the mixed product.

The aldehyde is widely used in flavor compositions (see also Tolylaldehyde-glycerinacetal), mainly for imitation Cherry, Peach, Apricot, Almond, Coconut, Vanilla, etc. and in fruit, berry, Muscatel and spice compositions.

The concentration in finished products varies from 10 to 400 ppm.

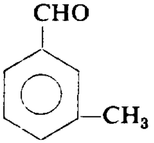
G.R.A.S. F.E.M.A. No.3068.

Prod.: by oxidation of mixed Tolylalcohols.

68-514; 106-340; 161-212;
See also monograph: *para*-Tolylaldehyde.

## 2960: meta-**TOLYLALDEHYDE**

*meta*-Methylbenzaldehyde.
*3*-Methylbenzaldehyde.
*meta*-Tolualdehyde.
*meta*-Toluic aldehyde.



$C_8H_8O = 120.15$

Colorless oily liquid. B.P. 200° C.
Sp.Gr. 1.02.

Almost insoluble in water, soluble in alcohol and oils.

Sweet and mild Benzaldehyde-type odor, less harsh, less penetrating and more tenacious than Benzaldehyde, but not as typical "almondy".

Since the title aldehyde is also less floral in its effect as compared to Benzaldehyde (which is used in traces in floral fragrances), and since it is many times more expensive than Benzaldehyde, there is no reason to believe that this aldehyde will become a very important one.

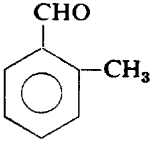
The material is rarely offered commercially, but the *para*-isomer is more commonly available (see monograph).

Prod.:
1) from *meta*-Xylene by oxidation.
2) from *meta*-Methylbenzylchloride by hydrolysis and oxidation.
3) from *meta*-Tolunitrile.

68-514; B-VII-296;
See also monographs: Tolylaldehyde-, *ortho*-Tolylaldehyde – and *para*-Tolylaldehyde.

## 2961: ortho-**TOLYLALDEHYDE**

*ortho*-Methylbenzaldehyde.
*2*-Methylbenzaldehyde.
*ortho*-Tolualdehyde.
*ortho*-Toluic aldehyde.



$C_8H_8O = 120.15$

Colorless oily liquid. B.P. 198° C.
Sp.Gr. 1.04.

Very slightly soluble in water, soluble in alcohol and oils.

Warm and sweet Benzaldehyde-type odor of moderate tenacity.

Apart from having a milder initial odor, no pungency, and slightly better tenacity, this aldehyde has little to offer over Benzaldehyde. It is more stable, but not very stable under mildly alkaline conditions, and it costs several times as much as Benzaldehyde.

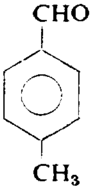
It finds a little use in perfume compositions, but the *para*-isomer is generally considered more interesting.

Prod.:
1) from *ortho*-Xylene by oxidation.
2) from *ortho*-Methyl benzylchloride by hydrolysis and oxidation.
3) from *ortho*-Tolunitrile.
4) from *ortho*-Xylylbromide plus Nitropropane in presence of Sodium ethoxide.

68-514; 100-1052; B-VII-295;

## 2962: para-TOLYLALDEHYDE

*para*-Methylbenzaldehyde.
*4*-Methylbenzaldehyde.
*para*-Tolualdehyde.
*para*-Toluic aldehyde.



$C_8H_8O = 120.15$

Colorless oily liquid.
B.P. 204° C. Sp.Gr. 1.02.

Very slightly soluble in water, soluble in alcohol and oils.

Warm and mildly floral, sweet-spicy odor of Benzaldehyde-type, but more floral and tenacious, less penetrating or harsh.

Sweet and warm fruity-Cherry, Bitter-almond type taste in concentrations near 50 ppm.

The title material is the most popular of the three isomers, but it is higher priced than the commercially available isomer-mixture (see Tolylaldehyde). It is more stable than Benzaldehyde, but it will eventually oxidize in air and deteriorate under alkaline conditions. As a minor ingredient in Cherry-blossom (mostly a fantasy-fragrance) or Lilac, Lily, Muguet, Rose, etc. it is quite popular for its lifting and sweetening effect. It has a "repairing" effect upon Anisaldehyde, which is commonly available in a rather mediocre fragrance quality, rarely as an impeccable, olfactorily pure quality.

Larger amounts are used in flavor compositions, partly as a modifier for Benzaldehyde, partly as a sweetener in fruity complexes, Cherry flavor, Coconut, etc.

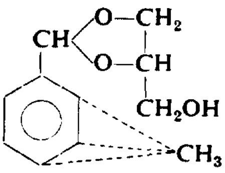
Prod.: from Toluene with Carbon monoxide and Hydrochloric acid in the presence of Aluminum chloride and Cuprous chloride.

5-106; 31-58; 68-514; 28-655; 155-130; 163-48; 163-73; 163-219; 163-241; B-VII-297;

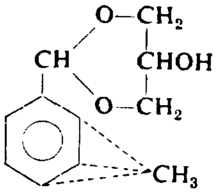
## 2963: TOLYLALDEHYDE GLYCERYLACETAL

"Tolyl glycerin".
Tolualdehyde glycerinacetal.

The commercial material is usually a mixture of the *1,2*-form and the *1,3*-form of the cyclic acetals of Glycerol with commercial Tolyl aldehyde, which is primarily *para*-Tolylaldehyde with some *ortho*- and *meta*-isomers:
(1) *2*-(*ortho*-*meta*-*para*-Cresyl)-*5*-hydroxymethyl dioxolan (about 60%) and
(2) *2*-(*ortho*-*meta*-*para*-Cresyl)-*5*-hydroxy dioxan (about 40%).



(1) main component.



(2)

$C_{11}H_{14}O_3 = 194.23$

Colorless, slightly viscous liquid.
Sp.Gr. 1.14. B.P. 292° C.

Slightly soluble in water, soluble in alcohol and most oils.

The material decomposes slowly in water, particularly in the presence of mild acids. The decomposition products are (mixed) Tolylaldehydes and Glycerol.

A very pure and freshly distilled material is practically odorless. It has a mild taste, and the Bitter-almond flavor develops usually during a taste test.

This acetal is used in flavor compositions, mainly for the purpose of "storing" Tolylaldehyde (see monograph) safely until immediately prior to need in the functional product. The material is capable of releasing all the Tolylaldehyde initially used in the preparation, and thus avoid loss by oxidation in the time spell until final use of the flavor. The acetal releases its aldehyde in contact with water and acids and under heat (baking, etc.).

Tolylaldehyde is preferred over Benzaldehyde for many purposes, mostly on account of its more spicy and less pungent-chemical aroma. It is used in imitation Chocolate, Cherry, Coconut, Vanilla, Almond, Pistacio, fruit complexes, etc. at concentrations from less than 1 ppm up to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.3067.

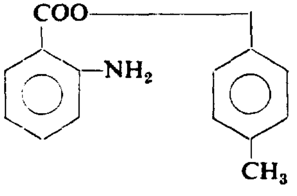
Prod.: from (mixed) Tolylaldehydes plus Glycerol with Phosphoric acid and using azeotropic distillation for water removal.

161-212;

## **2964:** para-**TOLYL ANTHRANILATE**

*para*-Cresyl anthranilate.

The commercial products, when available, has not been the Anthranilic ester with *para*-Tolylalcohol, but rather the Anthranilate of *para*-Cresol.



$C_{14}H_{13}NO_2 = 227.27$

Colorless or pale straw-colored, slightly viscous liquid. Sp.Gr. 1.15.

Practically insoluble in water, soluble in alcohol and oils.

Most commercial samples have been relatively impure, and odors vary from very faint or mild, sweet Jasmin-like to pungent Orange-blossom-Grape-like, all with good tenacity.

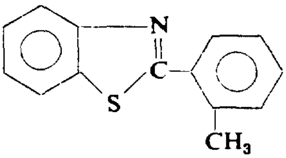
It is quite possible that a high-grade material could interest many perfumers, but it is most conceivable that perfumers will live very happily without it. It does not contribute any sensational notes or effects to a composition, other than those obtainable with conventional materials. It is reasonable to assume that the title material is practically obsolete in perfumery.

Prod.: from Isatoic anhydride and *para*-Cresol.

34-1011; 163-241;

## 2965: 2-TOLYL BENZOTHIAZOLE

*ortho*-Methyl-*2*-phenyl-(*1,3*-benzthiazole).



$C_{14}H_{11}NS = 225.32$

White crystalline powder. M.P. 108° C.
B.P. over 350° C.

Insoluble in water, soluble in absolute alcohol and most oils.

Very faint, but persistent leafy-rosy-musty odor. Like many other high-boiling, weak-smelling powders, it is very susceptible to odor contamination from processing or storage, and will easily adapt odors from exposure to odorous atmosphere.

The title chemical, a higher homologue to another rare item, slightly better known to the perfume industry, has been suggested for use as a fixative and modifier in Rose, Geranium and other fragrance types. Its effect can only be justly evaluated in actual use, and it may surprise many interested perfumers that the effect is quite perceptible at the level of 2 or 3%.

However, its solubility creates a problem, in that it is practically insoluble in diluted alcohol and therefore "banned" from use in certain perfume types. But since it is such a rare material, absent from most perfume laboratories, the problem may never occur.

In brief, the title material has some academic interest, but it is truly dispensable in the perfumer's daily "library" of working materials.

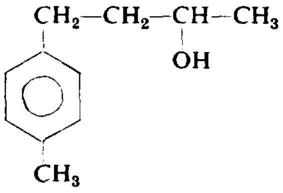
Prod.:

1) from *ortho*-Toluyl chloride plus *ortho*-Aminophenol.
2) from Sulfur and Benzyl methyl aniline.

69-427; 159-433;

## 2966: 4-(para-TOLYL)-2-BUTANOL

*2*-Hydroxy-*4*-(*para*-tolyl-)-butane.



$C_{11}H_{16}O = 164.25$

Colorless liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-green, powerful but natural odor, resembling the outer peel (rind) of Cantaloupe or Melon. Moderate tenacity.

Although the green-melony note of this alcohol is not nearly as powerful as that of certain unsaturated aldehydes or alcohols, it is unusually pleasant and relatively natural in its green character. This makes it a very handy and interesting perfume material, with which overdosage is not an immediate hazard.

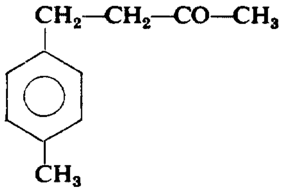
The material is rarely offered under its proper chemical name, but it was developed more than a decade ago by a company not specializing in perfume chemicals. "Green" materials have always had a bad reputation from a financial point of view, and most manufacturers will probably confirm, that this type of fragrance chemical is not the type most likely to bring profit to the chemical division. The volume is never large.

Prod.: by selective hydrogenation of *4*-(*para*-Tolyl)-*2*-butanone (see monograph next).

Sample: Dow Chemical Co., 1958.

## 2967: 4-(para-**TOLYL**)-2-**BUTANONE**

*para*-Methylbenzylacetone.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Very sweet, fruity-floral odor of good tenacity. The fruity notes are of Raspberry-Plum-like character, while the discretely floral notes have resemblance to the Gardenia fragrance.

Intensely sweet, deep-fruity taste in concentrations near 20 ppm. Perceptible at lower levels, and not objectionable at considerably higher levels.

The title material finds some use in flavor compositions as a modifier in Raspberry and other fruit imitation flavors, often as a partial substitute for *para*-Methoxyphenylbutanone, which is sweeter but milder, and other, related chemicals.

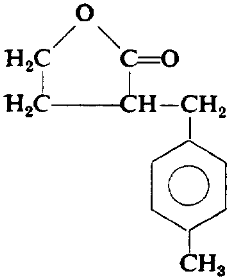
The ketone may be used in perfumery, but it is rarely offered commercially under its proper chemical name, although it is generally known in the flavor world under that name.

It could be used in Mimosa, Rose, Gardenia and other sweet-floral fragrances, variations of Jasmin, or in combination with Ionones in the conventional type lipstick fragrance.

Prod.: by condensation of *para*-Tolylaldehyde with Acetone, followed by hydrogenation.

G.R.A.S. F.E.M.A. No.3074.

## 2968: alpha-**TOLYL**-gamma-**BUTYROLACTONE**



(mostly *ortho*- and *para*-isomers).

$C_{12}H_{14}O = 174.24$

Colorless or pale straw-colored, viscous liquid. B.P. over 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Very faint, but very persistent sweet-balsamic, warm odor.

The odor has been described as "Tolu-balsam-like", but the author can not undersign that statement, and he believes it could be an error or "association" with the name "Tolyl-" which could subconsciously tempt an observer to find a Tolu odor.

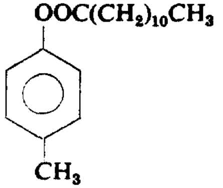
Actually, the material is included in this work mainly as an example of the "extreme" in Lactones, almost the end of the research line in this direction. Neither this material nor several of its lower homologues are of any substantial interest to the creative perfumer. Their "odor value" is negligible, and their odor character of little interest.

Prod.: (several methods) e.g. from Tolylmalonic ester and Ethylene oxide.

156-229; See also monograph: Benzyl butyrolactone.

## 2969: para-TOLYL LAURATE

*para*-Tolyl dodecanoate.
*para*-Cresyl laurate.
*para*-Cresyl dodecanoate (correct name).
The name "Tolyl-" is commonly used for this material.



$C_{19}H_{30}O_2 = 290.45$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

The title material is probably not used in perfumes. It is occasionally used in flavor compositions, but its odor is extremely weak, and its flavor mostly dependent upon the degree of hydrolysis by which *para*-Cresol is released.

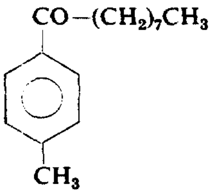
The flavor effect of the ester itself is mildly floral and sweet, but rather nondescript, and the author must admit that he can hardly see the effect or use of this material. The concentrations usually found in finished products are very low, about 1 to 2 ppm, and it is doubtful whether at this level the material can have any significant effect upon the overall flavor.

G.R.A.S. F.E.M.A. No.3076.

Prod.: from *para*-Cresolsodium and Laurylchloride.

## 2970: para-TOLYL-n-OCTYLKETONE

*para*-Methyl pelargophenone.



$C_{16}H_{24}O = 232.37$

White crystalline powder.

Practically insoluble in water, soluble in hot alcohol and oils.

Sweet-fruity, soft, but very tenacious odor.

Peculiar deep-fruity, Plum-Cherry-like taste in concentrations below 20 ppm. The taste is rather weak at this level, but higher concentrations seem to produce unnatural notes.

The title Alkyl-aryl-ketone has been suggested for use in perfume compositions, but it is very rarely, if ever, offered under its proper chemical name. It may find some use in certain perfume specialties, and bases, marketed under various trade names.

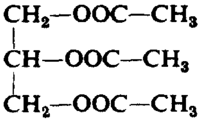
It may have been an offspring of research in line with the much more successful Benzyl dipropylketone (Morellone), which is widely used in flavors.

Prod.:
1) from Toluene and Nonanoyl chloride.
2) from *para*-Tolyl octylcarbinol by oxidation.

See also: 68-534;

## 2971: TRIACETIN

"Acetin".
Glyceryl triacetate.
"Enzactin".
"Vanay".



$$\begin{array}{l} CH_2-OOC-CH_3 \\ | \\ CH-OOC-CH_3 \\ | \\ CH_2-OOC-CH_3 \end{array}$$

$C_9H_{14}O_6 = 218.21$

Colorless, slightly viscous liquid. Sp.Gr. 1.16. B.P. 260° C.

7% soluble in water, miscible with alcohol and oils.

Very faint, ethereal-fruity odor, occasionally with acetic note (partly decomposed material).

Mild, sweet taste in concentrations lower than 500 ppm, but may appear bitter at higher concentrations.

The title material is not used as a flavor chemical or perfume material, but serves mainly as a solvent, mostly in flavors. It is often used in flavor types compatible with the mild taste of Triacetin, such as: Butter, Butterscotch, Nut flavors, spice blends, fruit complexes, etc.

Since the commercial marketing of Propylene glycol in high purity and at low cost has been followed by several other useful solvents, the need for Triacetin has declined, and the material is not used to the extent common in the 1930's or earlier. The material is very rarely, if ever, used as a solvent in perfume compositions.

G.R.A.S. F.E.M.A. No.2007.

Prod.: from Glycerin and Acetic anhydride, using Phosphoric acid or Zinc chloride as condensing agent.

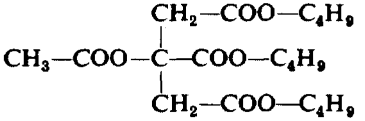
66-1024; 100-1056; B-II-147;

## 2972: TRIBUTYL ACETYLCITRATE

Acetyl tributylcitrate.

Citroflex A-4. (Chas. Pfizer Co.).

The Acetate of Tributylcitrate (see monograph).



$$\begin{array}{c} CH_2\text{—}COO\text{—}C_4H_9 \\ | \\ CH_3\text{—}COO\text{—}C\text{—}COO\text{—}C_4H_9 \\ | \\ CH_2\text{—}COO\text{—}C_4H_9 \end{array}$$

$C_{20}H_{34}O_8 = 402.49$

Colorless, slightly viscous liquid. B.P. over 300° C. Sp.Gr. 1.14.

Almost insoluble in water, miscible with alcohol and oils.

Very faint, sweet-herbaceous, winey-fruity odor.

An emulsion of the title material in water at 1000 ppm has only a very faint, mildly fruity-winey, berry-like odor and a mild, nondescript taste.

The title material is commercially available in a very high grade of purity, chemically, olfactorily and organoleptically.

Although it was originally designed for purposes of much larger volume use than perfumes and flavors, it has entered the flavor laboratory as a very useful solvent, co-solvent or "plasticizer" for materials which are non-miscible with the main flavor body, or for extracts, oleoresins, etc.

Its use in perfumery is very limited, because the perfumer has already a fairly wide choice of solvents at his disposal, while the flavorist has but very few.

Small amounts of the title ester are used in fruit flavors, mostly as blending note. The figures usually given for the concentration found in finished products are, however, in the author's opinion, too low. Concentrations lower than 1 ppm could not possibly have a perceptible effect upon the flavor of the finished product, and the author belives that concentrations up to 20 or 40 ppm are occasionally used, if not exceeded.

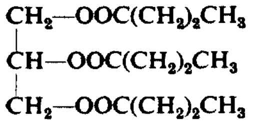
G.R.A.S. F.E.M.A. No.3080. Cleared by the American F.D.A. for use as a synthetic flavor and adjuvant.

Prod.: from Citric acid, via the Tributylester and by Acetylation to the title material.

66-1190; Sample: Chas. Pfizer Co. (USA).

## 2973: TRIBUTYRIN

Butyrin.
Glyceryl tributyrate.



$$\begin{array}{l} CH_2{-}OOC(CH_2)_2CH_3 \\ | \\ CH{-}OOC(CH_2)_2CH_3 \\ | \\ CH_2{-}OOC(CH_2)_2CH_3 \end{array}$$

$C_{15}H_{26}O_6 = 302.37$

Colorless, slightly viscous liquid.
Sp.Gr. 1.03. B.P. 308° C.

Practically insoluble in water, miscible with alcohol and oils.

Sweet, mildly fruity, buttery-creamy odor. Decomposed material shows dominating acid-butyric odor and loss of "creamy" aroma.

The taste is relatively bitter, practically to the minimum perceptible level, but the intensity of bitterness is not unpleasant even at concentrations in excess of 1000 ppm. The bitterness is easily overcome in the presence of sweetening agents plus acids.

The title material is not used in perfumery.

It finds some use in flavor compositions as a supporting blender for the more powerful flavor chemicals in imitation Butter (and Margarine) flavors, Butterscotch, Caramel, etc.

The concentration will be about 1000 ppm in candies, while it rarely exceeds 50 ppm in Margarine.

Prod.: from Glycerin and Butyric anhydride with a dehydrating agent or under conditions of azeotropic distillation of water.

G.R.A.S. F.E.M.A. No.2223.

66-1024; 100-1058; B-II-273;

## 2974: TRICALCIUM PHOSPHATE

Calcium phosphate, tribasic.
"Tertiary" Calciumphosphate.

$Ca_3(PO_4)_2 = 310.19$

Amorphous, white powder. M.P. 1670° C.

Insoluble in water, alcohol and oils. Soluble in diluted Hydrochloric acid or Nitric acid.

Odorless and tasteless.

The title material is briefly mentioned in this work, because it may be used in considerable amounts in dental powders, toothpaste, etc. as an abrasive, and in various food products as a "non-caking" agent. It is also used in certain beverages where the acidity is sufficiently high. Concentrations are up to 1000 ppm in beverages, about 50 to 100 ppm in other food products.

The title material is compatible with almost all known flavor materials and causes no great problem in that respect, but it may occasionally enhance the "musty" odor of Glycerin or Glycols, materials which are used in dentifrice preparations.

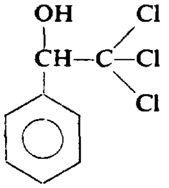
Dicalcium phosphate (Dibasic Calciumphosphate) is also used as an abrasive in dentifrices.

F.E.M.A. No.3081. G.R.A.S.

26-234; 100-137; 155-230;

## 2975: TRICHLORO METHYL PHENYL CARBINOL

Trichloro-*alpha*-phenylethylalcohol.



$C_8H_7OCl_3 = 225.52$

Colorless, slightly viscous liquid. B.P. 246° C.
Sp.Gr. 1.43.

Almost insoluble in water, soluble in alcohol and oils.

Very faint, metallic-green, musty-floral odor of good tenacity.

The title carbinol has not found much application in perfumery as such. Its esters, the Acetate in particular, are very well known (see following monographs).

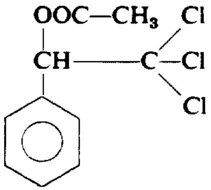
Apart from occasional use in "green-floral" fragrance types, such as Lilac, Gardenia, Jasmin, mainly inexpensive soap types, this material is of little interest and has very little odor value. In fact, it is very rarely offered commercially, even from the regular suppliers of the Acetate.

Prod.:
1) from Chloral with Aluminum trichloride in Benzene.
2) from Benzaldehyde and Chloroform.

5-69; 163-241;

## 2976: TRICHLORO METHYL PHENYL CARBINYL ACETATE

*1*$^2$, *1*$^2$, *1*$^2$-Trichloro-*1*$^1$-acetoxy-*1*-ethylbenzene.
Trichloro-*alpha*-phenylethylacetate.
The title material is mostly sold under trade name, and the most commonly used names are:
Abracador - Allorosal - Gerindol - Floranal - Rodalin - Rosone - Rosacetol - Rosetone - Rosamen - Rosephenone - Rosindol - Rosonone - Rose solide - Rosatol - Trirosol - Trirosal, etc. etc.
Many of the above trade names have been abandoned by the manufacturers, but are still used by perfumers for practical reasons (abbreviation).



$C_{10}H_9Cl_3O_2 = 267.55$

White crystalline powder or colorless crystals.
M.P. 88° C. B.P. 282° C.

Insoluble in water, somewhat soluble in alcohol, soluble in most perfume oils. The solubility in cold alcohol is sufficient for perfume composition purposes, but not to have a concentrated solution of the material on hand.

Mild, at first very weak, green-rosy, balsamic odor of excellent tenacity. The odor is much more perceptible when the material is in solution. There is some similarity to the odor of Benzophenone.

The title ester has found wide application in perfume compositions as a fixative in Rose and Geranium compounds, soap fragrances, powder perfumes, etc. because of its excellent stability and fixative effect. Its odor is better understood upon evaluation of Phenylethylalcohol with and without 5% of this material. There are still perfumers who find the title ester odorless or without any perfumery value, and it is sometimes because the material has been judged too hastily without a compounding experiment. Effective level is perhaps higher than 2%, but concentrations higher than 4% are rarely seen, although the material is inexpensive and freely available. The perfumer is simply satisfied with the effect, quite perceptible at that low level.

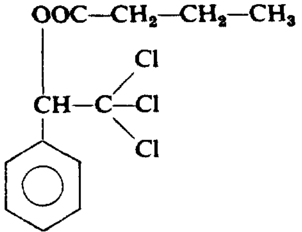
It is one of the very few chlorinated chemicals in common use in perfumes, and it has been popular ever since its discovery late in the 19th century.

Prod.: from the carbinol by Acetylation with Acetylchloride. See preceding monograph.

5-70; 33-516; 106-319; 163-74; 163-241;

## 2977: TRICHLORO METHYL PHENYL CARBINYL BUTYRATE

"Rosetone"-*n*-butyrate.
Trichloro-*alpha*-phenylethyl-*n*-butanoate.



$C_{12}H_{13}Cl_3O_2 = 295.61$

Colorless, slightly viscous liquid.
B.P. near 300° C.

Practically insoluble in water, soluble in alcohol and oils.

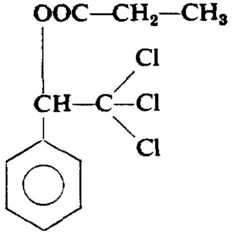
Very faint, sweet, green-balsamic, warm and very tenacious odor.

This ester is more of a curiosity than it is an important perfume material. It is very rarely offered commercially, and occasional samples have not aroused much interest among the perfumers. It lacks character, and its odor value is very limited. It is more expensive than the Acetate, and does not seem to offer better fixation.

Prod.: from the carbinol with *n*-Butyric anhydride.

## 2978: TRICHLORO METHYL PHENYL CARBINYL PROPIONATE

"Rosetone" propionate.
Trichloro-*alpha*-phenylethyl propionate.



$C_{11}H_{11}Cl_3O_2 = 281.58$

Colorless, slightly viscous liquid. B.P. 290° C. Sp.Gr. 1.31.

Practically insoluble in water, soluble in alcohol and oils.

Very faint, dry-rosy, warm and tenacious odor. The odor seems slightly stronger than that of the Acetate, and it could be that the fact that the Propionate is liquid, produces an impression of more odor.

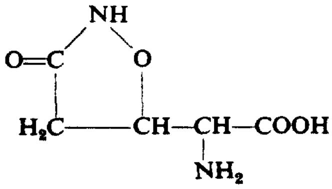
Of all the esters of Trichloromethylphenylcarbinol prepared since the successful Acetate, this is probably the only one of mentionable interest. The fact that it is liquid has some advantage – a sort of psychological advantage, since perfumers often subconsciously prefer a liquid material over a solid if the two have similar odor types and effects. At the same time, a perfumer will talk about "having need for more crystals in his compound", and actually referring to a type of fixation and background note, obtainable with certain liquid materials, too.

The title material is occasionally used as a fixative in Rose and Geranium fragrances, particularly for powder and soap, where its stability can be utilized.

Prod.: from the corresponding carbinol (see monograph earlier) with Propionic anhydride.

163-241;

## 2979: TRICHOLOMIC ACID



$C_5H_8N_2O_4 = 160.14$

White crystalline material.

Slightly soluble in water, soluble in diluted alcohol, poorly soluble in oils.

The title acid has been identified in and isolated from the Japanese fungus, Tricholoma muscarium, which in its natural state is known as a highly toxic plant.

Experiments with this acid and with the

closely related Ibotenic acid (see monograph) showed that these materials have outstanding synergistic effect upon the flavor of the so-called 5'-nucleotides (see Sodium guanylate and Sodium inosinate), and it has been established as a fact that the title material and its relative are powerful flavor potentiators.

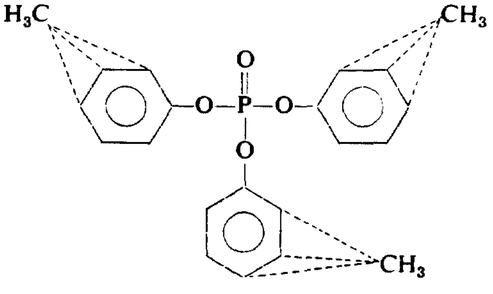
Research work on this subject continues, and it is still too early to make definite statements as to the future aspects of the title material, but it seems most likely that it will become a useful flavor "synergist".

Since these materials are effective at levels near 10 ppm (minimum) and since it has not yet been established whether the material itself is toxic, there is a good chance that it may become an approved flavor material.

157-519; 158-270;

## 2980: TRICRESYL PHOSPHATE

Tritolyl phosphate.
Celluflex.
Kronitex.
Lindol.
PX-917.
TCP.
The commercial product is usually a mixture of isomeric Tritolyl phosphates, although the individual isomers have industrial application.



$C_{21}H_{21}O_4P = 368.37$

Almost colorless, slightly viscous liquid.
Sp.Gr. 1.17. B.P. near 400° C.

Very slightly soluble in water, miscible with alcohol and oils, including mineral oil and vegetable oils.

The *ortho*-isomer is a liquid, while the *para*-isomer is a solid of M.P. 78° C.

The title material is briefly mentioned in this work because it has once accidentally been used in cooking oil for a large community of people. Airplane and other motor oils had been added to vegetable cooking oil, sold to Moroccan people along the West coast of Morocco in 1959. The motor oil contained the title material as an additive for lead-scavenging and other technical reasons, and it was not intended for human consumption. Thousands of local citizens consumed the cooking oil with the poison in it, and thousands became very seriously ill. Many hundreds were paralyzed for life, or crippled.

It has later been disclosed that the *ortho*-isomer of the above material is mainly responsible for such toxic effects, and one must hope that motor oil will never again find its way into a kitchen frying pan.

It is also of interest to note that the *ortho*-isomer is used in a newer synthesis for the production of Coumarin, via Chlorination followed by condensation with Acetic anhydride and Sodium acetate, e.g. in presence of Cobalt oxide catalyst.

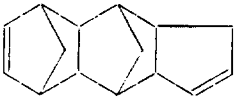
The commercial material is usually manufactured from Cresol (mainly from *para*-Cresol with Phosphorus pentachloride or Phosphor oxychloride. If the starting material is commercial "Tricresol", the product remains a mixture.

Needless to add, that the title material is not used in flavors or perfumes as such.

90-495; 90-593; 100-1062;

## 2981: TRICYCLOPENTADIENE

The commercial product (when available) consists mainly of the *endo*(=*alpha*-)-form, which is solid, with minor amounts of the *exo*(=*beta*-)-form, which is liquid.



$C_{15}H_{18} = 198.31$

White crystals or colorless, opaque, fused mass. M.P. 68° C. (*alpha*-isomer) B.P. 242°C.

Practically insoluble in water, soluble in alcohol and oils.

Peculiar earthy, mossy-musty odor, sweet-camphoraceous, warm and having some of the typical notes of Patchouli.

It also resembles the odor of Bicyclohexanone.

The title hydrocarbon has found some use in perfumery since it is very stable in soap, blends well with Oakmoss, Patchouli, Lavender, Opopanax, Ambregris materials, Sandalwood materials, etc.

It is rarely offered commercially under its proper name, and its chemically correct and complete name is too long and complicated to be remembered by any perfumer.

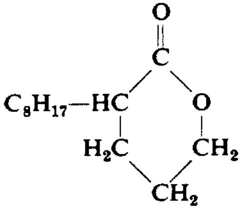
The last decade or two have brought a wide variety of camphoraceous and earthy and green odor chemicals to the perfume laboratory, and it is possible that the title material cannot keep up with this competition. It may be considered obsolete and of academic interest only. It is chemically related to the Indane musks.

Prod.: by Polymerization of Dicyclopentadiene, e.g. by heating. This hydrocarbon is obtained by self-condensation of Cyclopentadiene.

163-390; 67-345;

## 2982: delta-TRIDECALACTONE

*alpha-n*-Octyl-*delta*-valerolactone.
*delta*-Tridecanolide.



$C_{13}H_{24}O_2 = 212.34$

Colorless, viscous oil. Sp.Gr. 0.93.

Practically insoluble in water, soluble in alcohol and oils.

Soft, creamy, mildly coconutty and discretely musky odor (non-animal) of excellent tenacity.

Creamy, milky Coconut-like taste in concentrations lower than 5 ppm. Pleasant level is near 2 ppm. Concentrations higher than 20 ppm seem to produce bitter taste.

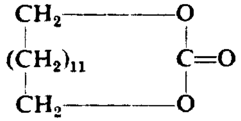
The title Lactone has only been commercially available for a few years, and it has rightfully attracted much interest. Its odor type is immediately inviting and stimulating to the alert creative perfumer, while the flavorist undoubtedly can find many ways of experimenting with this powerful chemical.

As a new and versatile modifier for the conventional Nonanolide/Undecanolide company in Gardenia and Tuberose, it can introduce the soft and sweet floral undertones with much more elegance, and the often dominating, fruity notes are subdued or not present. The title material blends very well with the macrocyclic musks or the Indane type musks, with Sandalwood, Lavender, Methylionones, Ambregris materials, etc., and although it may never become a "large-volume" perfume chemical, it may well become a standard resident on the perfumer's shelf.

Sample: Soda Aromatic Co., Osaka, Japan, 1967.

## 2983: TRIDECAMETHYLENE CARBOXYLATE

Tridecamethylene carbonate.



$C_{14}H_{28}O_3 = 242.36$

Colorless, slightly viscous liquid. Solidifies in the cold.

Almost insoluble in water, soluble in alcohol and oils.

Pleasant and rich, musky odor, slightly weaker than that of Tetradecamethylene carboxylate (see monograph), and less tenacious.

The title material has been suggested for use as a "macrocyclic musk", but since its manufacture is more costly than that of Tetradecamethylene carboxylate, there is not much reason to prefer the title material. It may have only academic interest now, while a few of its homologues are still in use – in competition with the many excellent macrocyclic musks developed during the past decade or so.

Prod.: from Tridecamethylene glycol and Butyl carbonate with Sodium, followed by decarboxylation by heat.

31-127; 156-261; 159-439;
See also comments under monograph: Tetradecamethylene carboxylate.

## 2984: TRIDECANAL

Tridecaldehyde.
Tridecyl aldehyde.
Aldehyde C-13.
(Some of the commercial materials are mixtures of several isomers, but the pure Tridecanal-*1* has also been prepared).

$CH_3(CH_2)_{11}CHO$

$C_{13}H_{26}O = 198.35$

Colorless oily liquid, solidifying in the cold. M.P. 14° C. B.P. 251° C.

Practically insoluble in water, soluble in alcohol and oils.

Polymerizes easily and will show floccules of white polymer in the liquid.

Powerful waxy, fresh-citrusy, Grapefruit-peel-like odor with slightly floral, petal-like waxy character and good tenacity.

The dry freshness has some resemblance to notes in the Ambregris complex.

This aldehyde, although not very common, has found use in perfume compositions for its power and freshness, equally useful in top-notes and in the heart of the fragrance. It combines delightfully with Oakmoss and Ambregris materials, with Ionones and Jasmin materials, etc.

It is often used in Honeysuckle and other heavy florals where it distracts from overly sweet, floral or fruity notes, while the tenacity of the fragrance is maintained.

Prod.: from Lauryl bromide, or from *n*-Dodecene via Oxo-reaction.

31-60; 66-477; 128-285;

## 2985: TRIDECANOIC ACID

Tridecylic acid.
Dodecan-*1*-carboxylic acid.

$CH_3(CH_2)_{11}COOH$

$C_{13}H_{26}O_2 = 214.35$

Colorless opaque mass or white crystals.
M.P. 44° C. B.P. 312° C. Sp.Gr. 0.85 (liquid).

Almost insoluble in water, soluble in alcohol and oils.

Very faint, waxy-woody odor. A highly purified material may be virtually odorless.

This acid has been suggested for use in Orris compositions and other perfume bases, but its effect is barely perceptible, and not always desirable. It was probably suggested originally because it had allegedly been identified in volatile oil or extracts from Orris rhizome, but the finding has not been confirmed.

In brief, it is a material of very little significance to the perfumer.

Prod.:

1) from Tridecylalcohol and concentrated Sodium hydroxide solution to yield Sodium tridecylate, from which the acid can be liberated.
2) from Dodecylbromide and Sodium cyanide via the Tridecylnitrile to the title acid by hydrolysis.

1-194; 66-564; 90-101; B-II-364;

## 2986: TRIDECANOL-1

*n*-Tridecylalcohol.
Alcohol C-13 (true).
A common commercial product is a mixture of isomers, all primary alcohols.

$CH_3(CH_2)_{11}CH_2OH$

$C_{13}H_{28}O = 200.37$

White crystalline mass or opaque waxy mass. M.P. 31° C. B.P. 262° C. B.P. for the mixed isomers is given at 276° C. Sp.Gr. 0.85.

Insoluble in water, soluble in alcohol and oils.

Very faint, waxy-woody and sweet-fruity odor of good tenacity. Although the material does impart a flavor to water or sugarwater, the taste impression is barely perceptible, and more like a mouthfeel (waxy) than a taste – at concentrations down to 10 ppm.

The title material has been used in certain perfume compositions, mainly artificial flower absolutes and a few bases.

It has also been suggested for use in imitation Banana flavor, since it has been identified as a natural component of Banana pulp. The flavorist has, however, many years before this discovery, used items such as Mimosa absolute for a similar effect in imitation Banana, and it could very well be that the effect of the Mimosa is due to the title material or a closely related chemical.

Prod.:

1) by reduction of Tridecanal-*1* from *n*-Dodecene-*1*.
2) by hydrogenation of Tridecen-*2*-al-*1* (see monograph) with Platinum catalyst in alcohol.

89-50; B-I-428;
Enjay data 1961; Union Carbide Chem. Co. data 1961;

## 2987: 2-TRIDECENAL

Tridecen-*2*-al-*1*.
*3*-Decylacrolein.

$CH_3(CH_2)_9CH{=}CH{-}CHO$

$C_{13}H_{24}O = 196.34$

Colorless oily liquid. B.P. 232° C.
Sp.Gr. 0.87.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, waxy-citrusy, peel-like odor of moderate tenacity. More citrusy than the odor of Tridecanal.

The title aldehyde is rarely used in perfumes, but it could find some application in complex Citrus topnote compositions, etc. It blends very well with Bitter Orange oil and Lime oil.

It is used in minute amounts in flavor compositions, mainly of the Citrus type, but also in fruit complexes, where it introduces great power, diffusion and lift to the aroma, reviving an overly sweet Citrus complex, etc.

The concentration in finished products is normally very low, about 0.1 to 8 ppm.

G.R.A.S. F.E.M.A. No.3082.

Prod.: from Undecyl aldehyde (Undecanal) by condensation with Acetic aldehyde, using Sodamide in Ether as condensing agent.

89-49;

## 2988: TRIDECYL ACETATE

Acetate C-13 (true).

$CH_3(CH_2)_{11}CH_2{-}OOC{-}CH_3$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid. Sp.Gr. 0.89.

Almost insoluble in water, soluble in alcohol and oils.

Mild, fatty-fruity odor of Peach-Apricot type with a Lily-floral note.

This ester has been suggested for use in perfume compositions, and may find a little use in topnote complexes for delicate floral fragrances, Citrus complexes, Chypres, etc. It blends well with the Citrus oils, with Clary Sage and Coriander, Bois de Rose, etc. and with many Orris materials. It is also a useful modifier for the alifatic aldehydes in aldehydic topnote compositions.

The ester is not listed as G.R.A.S. in the American index, but it could possibly find use, if approved, as a trace ingredient in imitation Banana, Peach, Apricot and Coconut flavor, or in certain fruit complexes.

Prod.: by azeotropic esterification of Tridecanol with Acetic acid.

33-502;

## 2989: TRIDECYLENIC ALCOHOL

*2*-Tridecen-*1*-ol.
Tridecenyl alcohol.
*3*-Decyl allylalcohol.
*3*-Decyl-*2*-propen-*1*-ol.

$CH_3(CH_2)_9CH{=}CH{-}CH_2OH$

$C_{13}H_{26}O = 198.35$

Colorless oily liquid, solidifying in the cold. M.P. 15° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful oily-citrusy odor of moderate tenacity.

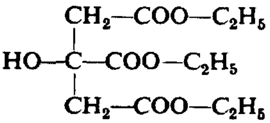
This alcohol has occasionally been commercially available and was sometimes used in Citrus type fragrances and perfume topnote bases, etc. The now available alifatic Dienols and Dienals have aroused more interest for this purpose, and, although they are still very expensive, they seem to be favored by the perfumers.

Prod.:

1) by selective reduction of Tridecenal (see monograph).
2) from Tridecylenic acid by hydrogenation.

## 2990: TRIETHYL CITRATE

Ethyl citrate.
Citroflex No. 2. (Chas. Pfizer Co., USA).



$$\begin{array}{l} \quad\;\; CH_2{-}COO{-}C_2H_5 \\ \quad\;\;\; | \\ HO{-}C{-}COO{-}C_2H_5 \\ \quad\;\;\; | \\ \quad\;\; CH_2{-}COO{-}C_2H_5 \end{array}$$

$C_{12}H_{20}O_7 = 276.29$

Colorless, slightly viscous liquid. B.P. 294° C. Sp.Gr. 1.14.

Practically insoluble in water, soluble in alcohol and oils.

Very mild, but sweet and pleasant, winey-fruity, Plum-like odor. The taste is bitter at concentrations higher than 500 ppm, but hardly perceptible at concentrations below 100 ppm.

The title ester was developed for purposes other than perfumery and flavor work, but it has become quite popular as a blender, solvent or diluent in perfumes and – particularly – in flavor compositions. The effect in a perfume composition is somewhat more than that of a diluent, since the ester, when blended with more volatile materials, does contribute a soft, mellow, warm-fruity undertone and often also a winey-sweet topnote to a fragrance. It is particularly interesting in Rose bases.

The ester is more commonly used in flavors, mainly in berry types, Butter, Butterscotch, Cherry, Honey, Citrus complex flavors or fruit flavors (particularly for fixation, for baked goods, etc.).

The concentration is normally about 10 to 50 ppm, but may be as high as 200 ppm in certain types of finished product.

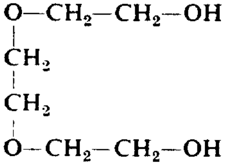
Prod.: by esterification of Ethylalcohol with Citric acid.

G.R.A.S. F.E.M.A. No.3083.

17-71; 17-170; 66-1190; 100-426; 159-407;

## 2991: TRIETHYLENE GLYCOL

Ethylene glycol-*bis*-2-hydroxyethylether.



$C_6H_{14}O_4 = 150.18$

Practically colorless, viscous liquid.

Sp.Gr. 1.13. B.P. 288° C.

Solidifies in the cold, melts again at minus 4° C.

Almost odorless, or having a faint, musty odor. The taste is bitter and acrid until the concentration falls below 20 ppm. It is barely perceptible at 5 ppm.

Miscible with water, alcohol and most oils, but not with hydrocarbons (e.g. Terpenes).

The material is hygroscopic.

This glycol has found some use as a solvent or diluent in perfume compositions, occasionally as a co-solvent for perfumes to be made water-soluble, etc. Also for industrial masking agents, technical perfumes, etc. to be made water-dispersible. It is not classified as a perfume material and it has only a depressing effect upon a fragrance and does not contribute positively as a fragrance material.

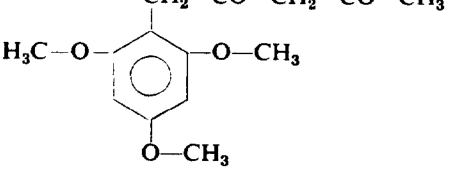
Since the glycol is considered about equal in toxicity to Ethylene glycol, it should not be used in flavor compositions at all.

Prod.: (many methods) e.g. from Ethylene oxide plus Ethylene glycol with sulfuric acid. This process also yields some Diethylene glycol and Tetra ethylene glycol.

66-667; 100-1063; B-I-468;
Union Carbide Chemicals Co. data.

## 2992: 2,4,6,-TRIMETHOXYBENZOYLACETONE

*5-(2,4,6*-Trimethoxyphenyl)pentane-*2,4*-dione.



$C_{14}H_{18}O_5 = 266.30$

Yellowish crystals.

Almost insoluble in water, soluble in alcohol, miscible with most oils.

Intensely sweet, warm-herbaceous odor, suggestive of Labdanum and Oakmoss.

The title material is rarely offered under its proper chemical name, but it has found use in perfume bases and specialties.

It is useful in floral as well as non-floral fragrance types, but its odortype suggests balsamic and non-floral types. It blends well with Labdanum, herbaceous oils, Lavender in particular, and it gives interesting effects when used with Coumarin and Oakmoss.

A considerable number of related materials have been prepared for possible use in perfume compositions, and many are still used under trade names, hardly known in most perfume laboratories.

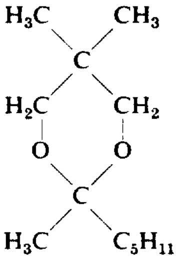
Prod.:

1) from Trimethoxybenzoyl chloride and Sodio-acetoacetic ester.
2) from Phloracetophenone and Ethylacetate, followed by Methylation of the resulting Trihydroxy benzoylacetone.

68-755;

## 2993: 2,5,6-TRIMETHYL-2-AMYL-1,3-DIOXANE

Methyl-*n*-amyl ketone-*2,2*-dimethyl-*1,3*-propanediol ketal.



$C_{12}H_{24}O_2 = 200.32$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful oily-fruity, heavy-floral, sweet odor of moderate tenacity. It is, as always in these condensation products, of paramount importance that the material is "well balanced" chemically, in other words, prepared with a minimum of surplus of the more powerful parent ingredient. In this type of cyclic acetal and ketal, one parent component is practically odorless, and the elimination of surplus of the other ingredient is therefore usually achieved by introducing a surplus of the odorless parent, which can be washed away with water at the completion of the process.

A very pure material is extremely interesting and should have good possibilities in perfumery as a "new note" in Gardenia, Ylang, Lilac, Musk compositions and the almost "classic" Musk-Peach-theme. In Lavender-Fougères it gives power and freshness.

The title material represents a large family of relatively new perfume materials developed from simple aldehydes or ketones with commercially available glycols.

Prod.: by condensation of Methyl-*n*-amyl ketone with *2,2*-Dimethyl-*1,3*-propanediol.

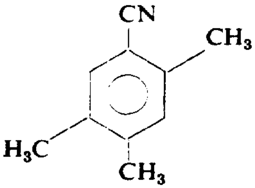
The product from Methyl-*iso*-amyl ketone is known, but it has a rather unnatural and harsher note.

The product from Methyl hexyl ketone has a powerful fatty-floral, nut-like odor with a buttery tone, useful in Gardenia, Tuberose, Orris, etc.

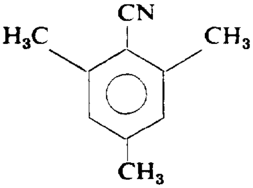
See also: *5,5*-Dimethyl-*2-n*-amyl-*1,3*-dioxane. Perfumery and Essential Oil Record, July 1966, pages 427-433;

## 2994: TRIMETHYL BENZONITRILE

*2,4-5*-Trimethyl phenylcyanide (structure I) and
*2,4,6*-Trimethyl phenylcyanide (structure II).
Other isomers are known, but rare.



I: Durylic acid, nitrile.
Durylonitrile. M.P. 57° C.



II:
M.P. 55° C.

$C_{10}H_{11}N = 145.21$

White or colorless crystals.

Very slightly soluble in water, soluble in alcohol and oils.

Peculiar, pungent-warm, Nut-like and earthy odor of considerable tenacity.

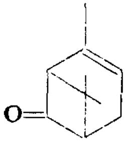
The title material(s) are briefly mentioned here because of their potential interest to perfumery. They have been suggested for use in Oakmoss compositions, but are very rarely offered under their proper chemical name. Most conceivably, they are incorporated in various bases and artificial Oakmoss specialties.

They are produced from Pseudo-cumene or Mesitylene, respectively, and the corresponding aldehydes are also known and interesting to perfume chemistry.

68-544;

## **2995:** 1,1,7-**TRIMETHYLBICYCLO**-(1,1,3)-**HEPTEN**-1-**ONE**

"Chrysanthenone".
(Formerly called "Carene epoxide").



$C_{10}H_{14}O = 150.22$

Colorless or pale straw-colored, oily liquid.
Sp.Gr. 0.95. B.P. 191° C.

Practically insoluble in water, soluble in alcohol and oils.

Warm-herbaceous, powerfully "dark"-green or "bitter"-green odor of moderate tenacity. The greenness resembles that of cut flower stalks, or freshly cut Chrysanthemums.

This ketone, an isomer of Verbenone (see monograph), has been suggested for use in perfume compositions, particularly in fragrances for household products and other low-cost fragrances. However, since it is normally manufactured from Verbenone, it is more expensive than that material, and they are not yet widely used or commonly used in fragrances.

The material is also interesting from a chemical point of view, in that it represents a group of fragrance chemicals, almost new to the perfumer, although not to the research chemist, and it is most conceivable that we will see many related chemicals offered as fragrance materials in the near future.

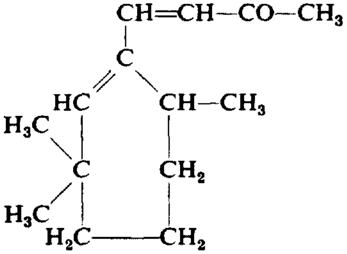
Its structural relationship to *3*-Carene, which has become commercially available in quantity, is also interesting.

Prod.: from Verbenone by Isomerization under UV-light in a hydrocarbon solvent.

The title material is not chemically related to Ethyl chrysanthemumate (1187), see that monograph.

89-348;
See also: Journal of The Chemical Society (London) 1960, pages 28 to 64 (J.J. Hearst and G.H. Wood).

## **2996:** 4-(2,6,6-**TRIMETHYL**-7-**CYCLOHEPTENYL**)-3-**BUTEN**-2-**ONE**



$C_{14}H_{22}O = 206.33$

Colorless or pale straw-colored, oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, sweet-woody, Orris-Violet-like odor, more woody than *alpha*-Ionone, but softer and more tenacious than the average type Methyl ionone.

The title ketone, usually offered under trade name or as component of a specialty base, was developed many years ago during an extended research on new Ionone types, based upon a new type of aldehydes in place of Citral.

A number of these materials appeared to have interesting odor, but very few have remained in production as perfume chemicals. The availability and cost of the parent aldehyde is often a decisive factor in the economy of Ionones, and with the extremely hard competition from new methods of manufacturing Citral for Ionones, the older or the odd aldehydes have very little chance of surviving, unless they can offer very unusual odor quality.

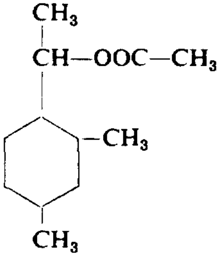
Prod.: by condensation of Acetone with *2,6,6*-Trimethyl-7-cyclohepten-*1*-al. (Swiss patents of Firmenich, 1934).

A great variety of isomers and related ketones have been prepared.

31-96;

## 2997: alpha-2,4-TRIMETHYL CYCLOHEXANE METHYLACETATE

Methyl-hexahydro-*2,4*-dimethylphenylcarbinyl acetate.



$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Powerful, green-fruity, but overall sweet and moderately tenacious odor.

The title ester, rarely offered commercially, has found a little use in perfumery, but the author feels that it is practically obsolete on account of failing interest.

The material adds power to the fruity-floral and mildly green notes of Jasmin or Rose, Gardenia and even non-floral fragrance bases, but it lacks character and is not very versatile.

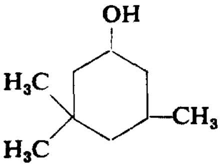
Prod.:

1) from *2,4*-Dimethyl acetophenone (which is commercially available) by hydrogenation, followed by Acetylation of the secondary alcohol.
2) from *2,4*-Dimethylbenzaldehyde via Grignard type reaction, followed by hydrogenation and Acetylation. Also from *2,4*-Dimethylcyclohexane carboxaldehyde, avoiding the hydrogenation.
   *2,4*-Dimethylbenzaldehyde is obtained from Pseudo-cumene by oxidation.

## 2998: TRIMETHYL CYCLOHEXANOL

*3,5,5*-Trimethyl cyclohexanol.
*3,3,5*-Trimethyl cyclohexanol.
*1*-Methyl-*3,3*-dimethylcyclohexanol-*5*.
Dihydro-*iso*-phorol.
"Cyclonol" (Interchem, Bush, etc.).

NOTE: Do not confuse the title material with Trimethyl hexanol (see monograph No. 3007).



$C_9H_{18}O = 142.24$

Translucent, colorless, fused mass, or crystals. M.P. 59° C. B.P. 198° C.

Almost insoluble in water, soluble in alcohol and oils.

Powerful Menthol-like odor, but more camphoraceous, less cooling than Menthol.

Camphoraceous-Menthol-like taste, but with little cooling mouthfeel at concentrations where Menthol has conspicuous cooling effect (about 50 ppm and higher). Overall coarser, but in suitable dilution quite pleasant taste without bitterness.

The title material became interesting to the flavor industry shortly after World War II, when, after a brief spell of incredibly low market price, Menthol became very expensive.

The "Cyclonol" found extensive use as a partial replacement for Menthol in toothpaste flavors, candy and chewing gum. The material was never included in the American G.R.A.S. list.

Since it is now a common industrial chemical, priced at about one-third of normal Menthol market cost, it has found further use in perfume compositions for household products, room sprays, detergents, cleansers, etc. and in various low-cost fragrances. It will enhance the entire fragrance if used at discrete level (between 0.5 and 2% usually) and give impression of more power, give radiance and "lift", even to floral fragrance types.

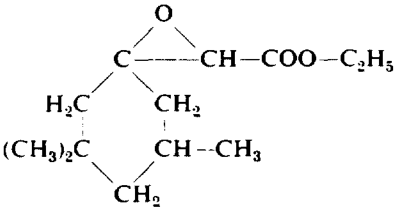
At the present cost, it has hardly any competition for its particular effect, and it may have a good and long future in modern perfumery for low-cost fragrances and the like.

Prod.: by complete hydrogenation of *iso*-Phorone (see monograph).

Dehydration of the title material with Zinc chloride yields *alpha*-Cyclogeraniolene (*1,5,5*-Trimethylcyclohex-*1*-ene.).

28-544; 67-145; 67-160;

## 2999: 3,5,5-TRIMETHYLCYCLOHEXANONE ETHYLGLYCIDATE



$C_{13}H_{22}O_3 = 226.32$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and warm-herbaceous odor, suggestive of cured Tobacco leaves. Excellent tenacity.

The title ester has been suggested for use in perfume compositions. It represents one possibly successful material out of a series of research experiments based upon Cyclohexenone- and Cyclohexanone-derivatives.

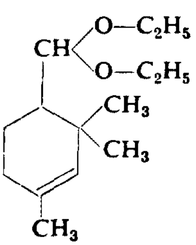
Since the title material is a relatively recent development, it is still too early to make statements of its future prospects in perfumes or flavors.

Prod.: from *3,5,5*-Trimethyl cyclohexanol (Cyclonol) by oxidation with Chromic acid. The resulting ketone is subsequently treated with Dibromo ethylacetate and Magnesium amalgam to yield the glycidic ester.

See also: 67-199;
Recherches, vol. 14, December 1964, pages 90-92 (Roure-Bertrand Fils et Justin Dupont, S.A.).

## 3000: 2,2,4-TRIMETHYL-3-CYCLOHEXEN-1-ALDEHYDE DIETHYL-ACETAL

*2,2,4*-Trimethyl-*1,2,5,6*-tetrahydrobenzaldehyde diethylacetal.



$C_{14}H_{26}O_2 = 226.36$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Powerful and very diffusive, green-bark-like, woody and mildly pine-like odor of moderate tenacity. The odor has been described as "Pine-sap-like".

This acetal is occasionally offered under trade name, rarely under its proper chemical name. It has been suggested for use in various perfume types, not only in Pine and Pine needle, but in Fougère, Wood, Chypre, etc. It performs well in bath oil perfumes and shampoos, and blends with Amylsalicylate, Oakmoss products, Cedarwood products, etc. for many types of low-cost fragrances.

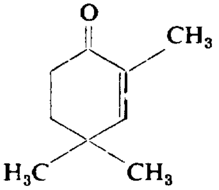
Prod.: from *2,2,4*-Trimethyl-*3*-cyclohexenaldehyde (which is an isomer of Cyclocitral, but not the commercial *iso*-Cyclocitral) by condensation with Ethyl alcohol or with Ethyl-*ortho*-formate with traces of mineral acid catalyst.

159-412;

A very large number of Cyclohexene carboxaldehydes and their derivatives were prepared in a research program by Dow Chemical Company in 1954 to 1959. The aldehyde corresponding to the title acetal was one of them.

## **3001:** 1,1,3-**TRIMETHYL**-2-**CYCLOHEXENONE**-4

*2,4,4*-Trimethyl-*2*-cyclohexen-*1*-one.



$C_9H_{14}O = 138.21$

Pale yellowish, mobile liquid. The color of aged material is often darker, and the viscosity higher, particularly after exposure to daylight.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful and rather pungent, but in dilution pleasant, warm-herbaceous and minty-camphoraceous odor, reminiscent of Tansy oil or Dalmatian Sage oil.

The title ketone has been suggested for use in perfume compositions, and if it became available in a state of higher olfactory purity and quality, it could well be used in modern soap and detergent fragrances, perfumes for household products, etc.

Its power and stability, and its low cost could make it a very useful "industrial" perfume chemical with a multitude of uses, including masking of objectionable odors.

It is an isomer of *iso*-Phorone (see that monograph) from which many interesting perfume chemicals have been developed.

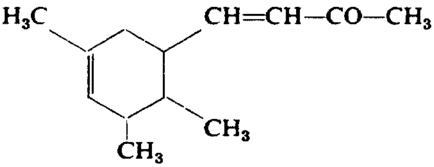
Prod.: as an industrial chemical from the Petrochemical industry. One method includes a Diene adduct (Diels-Alder) to a branched-chain ketone.

31-87; 67-210; 67-199;

## **3002:** 4-(2,4,6-**TRIMETHYL**-3-**CYCLOHEXEN**-1-**YL**)-3-**BUTEN**-2-**ONE**

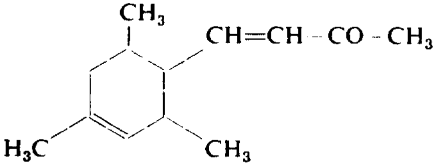
*2,4,6*-Trimethyl tetrahydrobenzalacetone (and isomers).
"Iritone" (I.F. & F.).
"Velvetine" (Dow Chemical Co.).
and many other trade names. See NOTE below.

The commercial products are usually mixtures of several isomers. The structures below and the text describe a product consisting mainly of:



*meta*-form.

and:



*symmetric*-form.
(Corresponds to title name).

$C_{13}H_{20}O = 192.30$

Pale straw-colored, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Soft-woody, sweet, balsamic-floral, tenacious odor. Products from different suppliers show considerable difference in odor characteristics.

The title material was introduced in the early 1950's but did not quickly interest the perfumers. And still today it is not widely used, although it forms component of many bases and specialties, and it is offered under its proper chemical name.

The main drawback is perhaps, that the material is not very versatile in its use, it resembles the Ionones too much, and is priced about the same as Ionones. The softness is sometimes translated as weakness in odor, but the material can only be justly evaluated for its effect in a composition, compared to the effect of Ionone in the same composition.

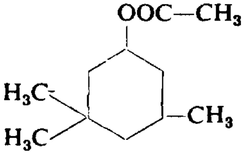
Prod.: from *iso*-Cyclocitral by condensation with Acetone. *iso*-Cyclocitral-S (= symmetric) yields the symmetric isomer.

Samples: Dow Chemical Comp. and I.F.&F. Inc.

NOTE: A commercially available product, claimed to be *2,5,6*-Trimethyl-*1,2,5,6*-tetrahydrobenzalacetone, is believed to be a product very similar to the title material (an isomer). It would be derived from an asymmetric *iso*-Cyclocitral.

## 3003: TRIMETHYL CYCLOHEXYL ACETATE

*3,5,5*-Trimethylcyclohexanyl acetate.
"Cyclonol acetate" (Interchem/Greeff).
NOTE: Do not confuse with: Trimethyl hexyl acetate (see monograph).



$C_{11}H_{20}O_2 = 184.28$

Colorless, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild, sweet-minty, herbaceous odor of moderate to good tenacity.

The title ester has been commercially available for many years, but has not been very successful in obtaining a space on the perfumer's shelf. The first impression of the odor of this material is an impression of weakness, which could be misjudged. The material is capable of adding life to herbaceous fragrances, sweetness and depth to Fougères and various types of non-floral fragrances. It is also of interesting effect in Rose compositions. Its low cost should be kept in mind, since it allows for liberal use of the material in fragrances for household products, etc.

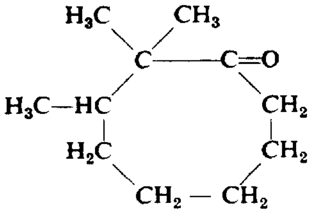
The material has been pointed out for its possible use as a part-adulterant in Lavandin oil in 1967-crops from France.

The title ester is not mentioned in connection with flavors and not listed as G.R.A.S. in the USA, but it could find use as a modifier for the alcohol (see Trimethyl cyclohexanol) in Mint types, provided the use of these materials became officially approved.

Prod.: by Acetylation of Trimethyl cyclohexanol.

Samples: Interchem corp./R. W. Greeff & Co., USA.

## 3004: 1,1,8-TRIMETHYL-2-CYCLO-OCTANONE



$C_{11}H_{20}O = 168.28$

Almost colorless, oily liquid.

Insoluble in water, soluble in alcohol and oils.

Warm-woody, sweet and tenacious odor of considerable resemblance to the Ionone type odors.

The title material has been suggested for use in perfume compositions and it is briefly mentioned in this work as an example of a series of perfume materials, developed under patent, of this unusual structure.

The material has been used in specialties, but is not offered commercially under its proper chemical name. Since it has been known for well over 30 years, and is still not widely used, one may conclude that it is nearly obsolete.

Prod.: from Trimethyl azelaic acid. (Firmenich French patent 744343).

31-86; 67-266;

## 3005: TRIMETHYL-ortho-FORMATE

Methyl-*ortho*-formate.
Trimethoxy methane.

$CH(OCH_3)_3$

$C_4H_{10}O_3 = 106.12$

Colorless mobile liquid. B.P. 102° C.

Slightly soluble in water, miscible with alcohol and oils.

Very diffusive, ethereal, pungent or nauseating odor, pleasant in dilution, slightly winey-fruity, Brandy-like.

Sweet taste in concentrations below 100 ppm. Barely perceptible at 10 ppm.

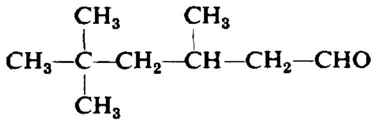
The title material has found a little use in perfume compositions for the powerful "lift" and the winey-ethereal topnote it can introduce. It will add mellowness to an alcoholic solution (Colognes, etc.) and give impression of completed ageing. Minute traces are used in flower bases, but the title material suffers from being chemically reactive with Aldehydes, Ketones, Acetoacetates and many other materials, possibly used in a perfume composition. One of its possible breakdown products is Methylformate, which is extremely volatile and will produce a powerful, not unpleasant, but certainly undesirable topnote. This effect is often concealed in Cologne-strength solutions of a fragrance.

Prod.: from Chloroform and Sodium methoxide in Methanol (Williamsons synthesis).

1-221; 65-554;

## 3006: 3,5,5-TRIMETHYL HEXANAL

"*iso*-Nonylaldehyde".
*tertiary*-Butyl-*iso*-pentanal.



$$CH_3-\underset{CH_3}{\overset{CH_3}{C}}-CH_2-\overset{CH_3}{CH}-CH_2-CHO$$

$C_9H_{18}O = 142.24$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very powerful and diffusive, dry-green, gassy odor, in extreme dilution refreshingly vegetable-green ("aldehydic"), yet dry and slightly woody, of moderate to poor tenacity.

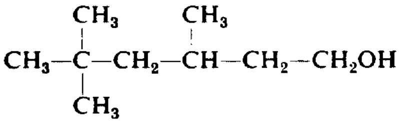
The title aldehyde has been suggested for use in perfume compositions as a very powerful masking agent. In extreme dilution, its odor is generally considered pleasant, but the opinion is not unanimous.

Partly on account of its very low cost, this material has found extensive use as the main active ingredient in various types of masking odors, room fresheners, deodorizers, etc. It is relatively stable against oxidation and polymerization, but it will produce intensely yellow colored condensation products with Anthranilates, darker with Quinolines or Indoles. However, it is rarely used in connection with those materials, more often with alifatic aldehydes, Monoterpenes, Pine fragrance materials, etc.

Prod.: (several methods) e.g. from Di-*iso*-butylene via Oxoreaction.

## 3007: TRIMETHYL HEXANOL

"*iso*-Nonyl alcohol".
*tertiary*-Butyl-*iso*-pentanol.
*3*,*5*,*5*-Trimethylhexan-*1*-ol.
Trimethyl hexylalcohol.
NOTE: Do not confuse with Trimethyl cyclohexanol (see monograph).



$$CH_3-\underset{CH_3}{\overset{CH_3}{C}}-CH_2-\overset{CH_3}{CH}-CH_2-CH_2OH$$

$C_9H_{20}O = 144.26$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Relatively powerful, oily-herbaceous, in dilution sweet odor, but not nearly as floral as *n*-Nonylalcohol. The overall impression is that of a "chemical" odor, rather nondescript, hard, and, unless highly diluted, not very pleasant.

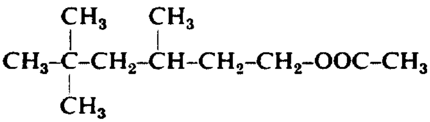
The material is marketed as an industrial chemical, but it is, from a chemical point of view, very pure.

It is rarely used as such in perfumes or flavors, but it is mentioned in this work because of the considerable interest the perfume industry has had in the corresponding aldehyde, and, to a lesser degree, in the Acetate of this alcohol, see the succeeding monograph.

Prod.: (many methods) e.g. from the Olefin by hydration, by chlorination of the hydrocarbon, followed by hydrolysis, by reactions involving Potassium-*tertiary*-Butoxide, etc. etc. It may also be obtained very inexpensively from Di-*iso*-butylene via Oxoreaction to the aldehyde, from which this alcohol is prepared by hydrogenation.

## 3008: 3,5,5-TRIMETHYL HEXYLACETATE

"*iso*-Nonylacetate" (Haarmann & Reimer)
"Vanoris" (I.F. & F.)
and many other trade names.
NOTE: Do not confuse with: Trimethyl cyclohexyl acetate (see monograph).



$$CH_3-\underset{CH_3}{\overset{CH_3}{C}}-CH_2-\overset{CH_3}{CH}-CH_2-CH_2-OOC-CH_3$$

$C_{11}H_{22}O_2 = 186.30$

Colorless liquid.

Practically insoluble in water, soluble in alcohol and oils.

Woody-fruity, soft, refreshing odor of mild Orris-type, more fruity and discretely green, with moderate tenacity.

The title ester had been known for many years before it was finally offered under its proper chemical name, but it never seemed to be able to arouse the interest of the perfumer. Yet the material has most of the virtues and prerequisites for success in fragrance chemicals:

It is relatively inexpensive – slightly higher than Linalyl acetate, and could be used at concentrations from 1 or 2% up to 6 or 8% under normal conditions, including soap fragrances. It might be considered for much higher concentrations if it were sold at a lower-cost. The ester is stable in soap and compatible with all conventional fragrance materials.

Its odor type is compatible with many floral types and with all woody fragrance types, in fact, it has often been compared to the odor of *para-tertiary*-Butyl cyclohexanyl acetate, a "volume" fragrance chemical sold at slightly lower price.

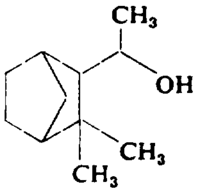
In spite of all its advantages, this ester is still unknown to many perfumers, absent from many perfume laboratories. One may add, that it does not have a very unusual odor, but this is rarely a drawback for a potential soap perfume chemical.

Prod.: from Trimethylhexanol (see monograph) by Acetylation.

Samples: I.F. & F. and H. & R.

## **3009:** alpha-3,3-**TRIMETHYL**-2-**NORBORNANE METHANOL**

Dihydro methylcamphene carbinol.



$C_{11}H_{20}O = 168.28$

Colorless viscous liquid, solidifying in the cold to an opaque crystalline mass.

Practically insoluble in water, soluble in alcohol and oils.

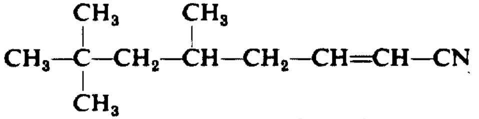
Sweet-woody, slightly oily and discretely piney odor of moderate tenacity. The resemblance to Sandalwood is not striking, but the effect in compositions suggests that the material can be used as a Sandalwood type fragrance chemical.

A considerable number of related chemicals have been developed during the past decade, and a few have become successful Sandalwood materials. The title material is, in the author's opinion, not likely to maintain any interest as such type of fragrance material against the competition from much more effective and true-to-Nature chemicals.

See also monographs:
Dimethyl norbonane ethanol (1028),
Hydroxyethyl bornanylether (1744),
Camphenyl methylpropanol (563),
Bornyl methoxy cyclohexanol (360).

Prod.: from Cyclopentadiene and Methyl ethyl ketone.

## **3010:** 5,7,7-**TRIMETHYL**-2-**OCTENYL NITRILE**



$$CH_3-\overset{CH_3}{\underset{CH_3}{C}}-CH_2-\overset{CH_3}{CH}-CH_2-CH=CH-CN$$

$C_{11}H_{19}N = 165.28$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

Powerful, oily-musty odor, suggestive of Leather and Oakmoss, in dilution more refreshing, remotely Ambre-like.

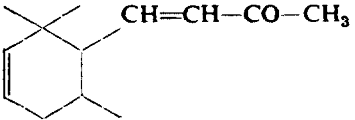
The title Nitrile is rarely offered under its proper chemical name, but it has been developed in search of new and interesting Nitriles, since the more successful Nitriles, equivalent to well-known Aldehydes, had been prepared and made commercially available.

The subject material has a very limited field of application, and although it has been known for many years, it has no success to prove that it will remain on the perfumer's shelf. Except for occasional and mostly experimental use in new Fougères, Men's fragrances, Citrus colognes, etc., the material may well be on its way to oblivion.

Prod.: by condensation of Trimethyl hexanal (see monograph) with Acetaldehyde, via the Aldoxime of the condensation product and by dehydration to the title material.

## 3011: 2,6,6-TRIMETHYL-1,2,3,4-TETRAHYDROBENZALACETONE

*4*-(*2*,*6*,*6*-Trimethyl-*4*-cyclohexenyl)-*3*-buten-*2*-one.
An isomer of Ionone.



$C_{13}H_{20}O = 192.30$

Colorless or pale straw-colored oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Sweet-balsamic, powdery, moderately tenacious odor of delicately woody character.

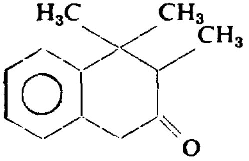
The title material may not be offered as such or under its proper chemical name, but it has found considerable interest as a component of various perfume specialties, often in combination with Ionones and Methylionones.

Its effect is mainly that of enhancing the powdery character, and supporting the soft-mellow undertones in such specialties, often recommended for powdery perfume types, and frequently used in very considerable proportions in perfume compositions of the more luxurious type.

Prod.: by condensation of Acetone with *2*,*6*,*6*-Trimethyl-*4*-cyclohexene carboxaldehyde. The aldehyde is an isomer of Cyclocitral.

## 3012: 1,1,2-TRIMETHYL TETRALONE-3

*3*,*4*,*4*-Trimethyl-*1*,*2*,*3*,*4*-tetrahydro-*beta*-naphthalone.



$C_{13}H_{16}O = 188.27$

Colorless viscous liquid, solidifying in the cold.

Practically insoluble in water, soluble in alcohol and oils.

Warm, slightly musty, dry-sweet Sandalwood-like odor with an Ambregris note and excellent tenacity.

The title material is not offered commercially as such, but perhaps in compositions with other materials in perfume bases and specialties.

It was developed at a time when Sandalwood-smelling chemicals were still rare, before the Camphanyl- and Camphenyl-derivatives appeared commercially. It is most likely that the subject ketone has lost its importance in perfumery and that it can be considered as practically obsolete.

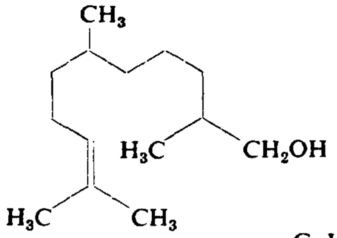
If it were available at a much lower cost, it could be included in Ambregris specialties, because it has an odor very compatible with the Ambregris olfactory picture.

Prod.: (several methods) e.g. by Friedel-Craft's synthesis from the corresponding acid chloride.

See also monographs:
*iso*-Bornyl methoxycyclohexanol (360).
*8*-*tertiary*-Butyl-*alpha*-benzosuberone (406).
*8*-*tertiary*-Butyl-*5*-methyl-*alpha*-tetralone (497).
*7*-*tertiary*-Butyl-*alpha*-tetralone (535).
*5*-Methyl-*7*-methoxy-*8*-*iso*-propyl-*alpha*-tetralone (2105).
*3*-Methyl-*4*(*4'*-*iso*-propylcyclohexyl)-butan-*2*-one (2217).

## 3013: 2,6,10-TRIMETHYL-9-UNDECEN-1-OL

Nor-tetrahydro farnesol.



$C_{14}H_{28}O = 212.38$

Colorless or very pale straw-colored, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

Intensely sweet, floral-balsamic and tenacious odor.

The title alcohol is rarely offered under its proper chemical name but it forms a major component of several successful specialties, and is generally used in discrete amounts in perfume compositions of the floral, balsamic, Oriental and powdery types.

It lends depth and warmth to a fragrance, mellows the topnote and softens overly aldehydic initial notes, briefly acts as a "liaison" between the topnote and the heart of the fragrance in many such cases.

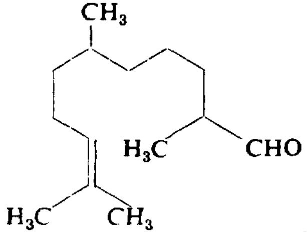
It gives interesting and pleasant effects in Muguet, Magnolia, Cassie, Sweet Pea and other florals, and it performs well with Sandalwood and with many of the carbinols.

Prod.: by Meerwein-Ponndorf-Verley reduction (with Aluminum-*iso*-propoxide) of the corresponding aldehyde, which is in turn obtained via Darzen's reaction upon Pseudo-ionone.

See also monograph: Trimethyl undecylenic aldehyde.

## 3014: TRIMETHYL UNDECYLENIC ALDEHYDE

"Adoxal" (Givaudan)
"Farenal" (Haarmann & Reimer).
Tetrahydro-nor-farnesal.
*2*,*6*,*10*-Trimethyl-*9*-undecen-*1*-al.



$C_{14}H_{28}O = 210.36$

Colorless or very pale straw-colored, slightly viscous liquid. Tends to increase viscosity upon standing, and will polymerize if exposed to air.

Practically insoluble in water, soluble in alcohol and oils.

Very powerful and very tenacious, sweet-floral, waxy-rosy odor, sometimes referred to as "ozone-like" (a very disputed odor description).

This aldehyde, known for several decades, has found wide application in perfume compositions for its power, sweetness and tenacity. It blends excellently with all Lily and Muguet-types, balsamic and Oriental fragrances (Sandalwood, Ionones, etc.), and with fruity types, including Gardenia, etc.

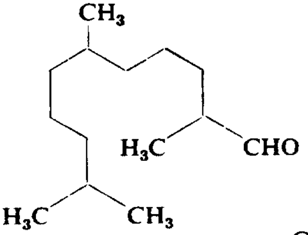
Originally promoted for use with the Ionones, it is now used in many modern types other than the Violet types or "heavy-Ionone" types. The power of this material is often underestimated, and it is necessary to study carefully the terminal notes of an experimental composition over an extended period in order to make certain that the concentration is perceptible, and not too high. Fractions of one percent may suffice in certain fragrance types, while concentrations up to 2% or more have been successful in the presence of suitable fixative components.

Prod.: from Pseudo-ionone via Darzen's reaction (Glycidate-intermediate).

106-24 (Givaudan data).
Haarmann & Reimer info.

## 3015: 2,6,10-TRIMETHYL UNDECYLIC ALDEHYDE

Trimethyl undecanal.
Nor-hexahydro farnesal.



$C_{14}H_{28}O = 212.38$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant, refreshing, floral-citrusy, rosy-aldehydic and slightly oily-fatty odor of moderate to good tenacity.

This aldehyde was introduced to the perfume laboratories many decades ago, and was also used under various trade names from European manufacturers. One of the originators was a chemical company, not in the perfume chemical business, but the material has stayed with the subsidiaries of that company, and related aldehydes and specialties have been developed from associated perfume chemical manufacturers.

In spite of its relatively long history, the title aldehyde has never become a truly "large" material, partly because it is extremely powerful and overdosage may easily occur in experimental perfumery, disappointing the perfumer, and possibly discouraging continued experimenting. The unsaturated, corresponding aldehyde, Trimethyl undecylenic aldehyde, has attracted more attention, and may eventually become the more popular of the series.

For accentuated floral effect, enhancing sweet-citrusy notes, refreshing of dull-woody notes, etc., the title aldehyde can find good application. But the author would predict a better future for the more intriguing and lively effects, and the versatility of, the unsaturated aldehyde (see preceding monograph).

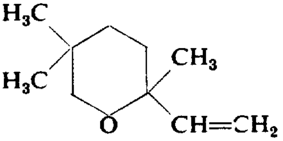
The title aldehyde has academic interest in showing that branched-chain aldehydes may have much stronger odors than the corresponding straight-chain alifatic aldehydes (compare Tetradecanal = Myristic aldehyde).

Prod.: by hydrogenation of Trimethyl undecylenic aldehyde.

2-1008; 31-39; 89-125;

## 3016: 2,2,6-TRIMETHYL-6-VINYL-TETRAHYDROPYRAN

An isomer of Rose oxide.



$C_{10}H_{18}O = 154.25$

Colorless mobile liquid. Sp.Gr. 0.86.
B.P. 160° C.

Almost insoluble in water, soluble in alcohol and oils.

The undiluted material has a sharp, almost irritating, but fresh-camphoraceous-cineolic odor, which becomes sweet, warm, herbaceous and pleasant upon dilution (near 1 %).

The title oxide, which has been identified in Geranium Reunion oil, has occasionally been commercially available, and it is likely that it will be regularly available in the future.

So far, it has mainly been used in artificial Geranium oils, a very fast growing item at the larger perfume houses, and in the perfume departments of the large soap companies.

A considerable number of Pyrans and related ethers or oxides have been investigated, synthesized and brought upon the perfumery market during the past few years. The problem was not solved with "Rose oxide" which – incidentally – is more than one chemical, and it appears that there may be many similar materials part-responsible for the power in the odor of Geranium, Rose and other essential oils.

Also known are:
*2*-Methyl-*4*-vinyl-*5*-*iso*-propenyl tetrahydropyran,
*2*-Methyl-*4*-vinyl-*5*-*iso*-propenylidene tetrahydropyran,
*2,6,6*-Trimethyl-*2*-vinyl tetrahydropyran.

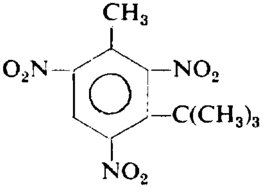
The latter is present in distilled Lime oil, and it is a very close isomer of the title material from Geranium oil.

It is interesting to compare the structure of the title material to that of *5*-Methyl-*3*-butyl tetrahydropyran-*4*-yl acetate (see monograph), which is primarily a Jasmin-type fragrance chemical.

163-379; 90-709;
See also: Recherches, vol. 14, Dec. 1964, page 96 (Roure-Bertrand Fils & Justin Dupont, Paris, France).

## 3017: TRINITRO-tertiary-BUTYLTOLUENE

"Musc Baur".
"Tonquinol".
*1,3,5*-Trinitro-*4*-pseudo-butyltoluene (abandoned name).
*2,4,6*-Trinitro-*3*-*tertiary*-butyltoluene.
Musk toluene.
*meta*-*tertiary*-Butyl-trinitrotoluene.



$C_{11}H_{13}N_3O_6 = 283.25$

Yellowish needle-like crystals. M.P. 97° C.

Moderately soluble in alcohol and most oils, almost insoluble in water.

Sweet, but rather coarse, musky odor of good tenacity.

This Nitromusk is included mainly for academic and historic reasons. The author believes that it is no longer used in perfumes, and perhaps no longer manufactured on a commercial scale.

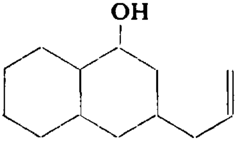
It represents the first, large-scale, commercially produced Nitromusk although Nitro-alkylbenzenes had been made earlier (Trinitro-*meta*-cymene was prepared by Kelbe in 1881), while the title material was developed in 1888, commercially available in 1890. A few years later it was superseded by Musk Xylol, a higher homologue. It is therefore the father of a Nitromusk still very much in use, and deserves mention. During the next 70 years, no Nitromusk was developed which was less expensive and equally (or more) versatile than Musk Xylol.

Prod.: from Toluene plus *tertiary*-Butylchloride and Aluminum chloride in a Friedel-Craft's reaction to produce the *tertiary*-Butyl derivative. Nitration with Nitric- plus Sulfuric acids yields the title material.

5-297; 95-198; 96-223; 159-633; 30-430; 31-194; 31-195;

## 3018: TUBEROL

*3*-Allyl-decahydro-*alpha*-naphthol.
*3*-(*2*-Propen-*1*-yl)-decalol-*1*.



$C_{13}H_{22}O = 194.32$

The title material is briefly mentioned in this work because of its repeated appearance – with very imperfect and unconfirmed data – in perfumery literature, and because of its total absence from the more authoritative sources and comprehensive works on the subject of odorous components of natural materials, synthetic perfume materials, etc.

The title alcohol and the corresponding ketone have been mentioned as important components of the volatile oil of Tuberose flowers. With the cost of natural extract (absolute) of Tuberose in mind, such information is bound to arouse interest.

But it has never been fully revealed, and reports of such substance being a (key) component in Tuberose have not been confirmed.

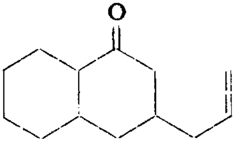
Various specialties under names such as the above, or closely related names, implying a relationship to Tuberose, have all been fragrance compositions, or "Tuberose perfumes".

Very little is known about the most important components of Tuberose fragrance (natural), but many of the odorous components have been identified. Most of these are very common esters: Methyl anthranilate, Methylbenzoate, phenylacetate, etc., while none of these indicate that the typical material(s) have been captured or identified yet.

See also next monograph: Tuberone.

## 3019: TUBERONE

*3*-(*2*-Propen-*1*-yl)-decalone-*1*.
*3*-Allyl-decahydro-*alpha*-naphthalone.



$C_{13}H_{20}O = 192.30$

See monograph: Tuberol, preceding this monograph.

The title ketone has been described as a "Tuberose principle" in perfumery literature.

However, the statement and findings have not been sufficiently supported by later confirmations or further analytical work.

The acetate of the corresponding alcohol would be Tuberyl acetate. A product under that name is commercially available from a perfume company whose founder published his finding of "Tuberone" 70 years ago.

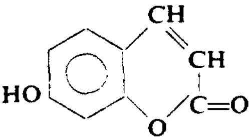
In view of the total lack of later confirmations, and in spite of the absence of contrary statements, it must be reasonably fair to assume that the title material can not be classified as the principle of Tuberose fragrance yet.

It would still be interesting to clarify this problem further.

See: Gildemeister-Treibs: Die Aetherischen Oele, Band IV, 455 (1956).

## 3020: UMBELLIFERONE

Skimmetin.
7-Hydroxycoumarin.



$C_9H_6O_3 = 162.15$

Colorless crystals. M.P. 224° C.

1 % soluble in hot water, poorly in cold water. Soluble in alcohol and in most oils. Alkaline, aqueous solutions show blue fluorescence.

Sweet-herbaceous, warm odor, very much resembling the odor of Coumarin, but not nearly as strong. Very tenacious.

The title lactone is very well known, but has not become important to the perfume industry as such. Its odor type suggests use parallel to that of Coumarin, but Umbelliferone is more expensive and causes some solubility problems. The "odor value" of Umbelliferone is also inferior to that of Coumarin.

Umbelliferone has found use as a sunscreening agent, because it absorbs UV light to a considerable degree. The phenomenon of fluorescence is related to its UV-light absorbing ability. It is probably of considerable value for this power in Nature, where Umbelliferone is found widely distributed. As for cosmetic preparations, newer sunscreens are now employed instead of Umbelliferone.

The material could still find use in perfume compositions as supporting note for Galbanum and Opopanax, in which it increases the sweetness and fixative power, and the lactone blends very pleasantly with Oakmoss products.

The Methylether, 7-Methoxycoumarin, is virtually odorless. It is also used as a sunscreening agent.

Prod.:

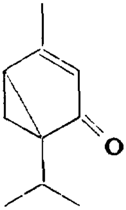
1) from *2,4*-Dihydroxybenzaldehyde plus Acetic anhydride by Perkin's reaction.
2) from Resorcinol and Malic acid with Sulfuric acid in a Pechmann-synthesis.

1-558; 31-167; 69-879; 90-599; 96-180; 100-1079; B-XVIII-27;

## 3021: UMBELLULONE

*4*-Methyl-*1*-*iso*-propyl-bicyclo(*0:1:3*)-hexen-*3*-one-*2*.

The title material is not related to Umbelliferone (see monograph).



$C_{10}H_{14}O = 150.22$

Colorless oily liquid. Sp.Gr. 0.94.
B.P. 211° C.

Practically insoluble in water, soluble in alcohol and oils.

Pungent and irritating, but in dilution rather pleasant, minty-Tansy-like, resinous-balsamic odor of moderate to poor tenacity.

The title ketone is harmful to the human mucous membranes, and it is toxic by ingestion. Nevertheless, it has been mentioned repeatedly in connection with perfume application. The author believes that this material does not have any highly desirable olfactory effect or other perfumery value except what could be achieved by means of safe and conventional materials, and the hazards of this material are simply too obvious to neglect.

Apart from some academic interest, the material should preferably remain a chemical in organic chemical research, and not arrive on the shelf in the perfume laboratory. Years ago, the ketone was used in a process for making Thymol (by oxidation or catalytic dehydrogenation).

Prod.: by isolation from the essential oil of Umbellularia californica (California laurel) in which the ketone is present at the rate of 20 to 60%.

The ketone may be accompanied by Pseudo-umbellulone, a solid isomer.

17-89; 65-440; 89-340; 163-242; 5-285;

## 3022: UNDECA-2,4-DIEN-1-AL

Octenyl acrolein.

$CH_3(CH_2)_4CH_2—CH=CH—CH=CH—CHO$

$C_{11}H_{18}O = 166.27$

Colorless mobile oil.

Practically insoluble in water, soluble in alcohol and oils.

Very powerful oily-caramellic, "baked-spicy" odor with citrusy undertones. A fragile aldehyde like this is likely to deteriorate rather quickly, and odor descriptions inevitably vary with the age and origin of the material.

It is extremely prone to acetal-formation, and its alcoholic solution soon produces the caramellic-vinous topnote characteristic of these acetals.

However, the oily-buttery, baked note seems to be indigenous to this aldehyde. It has only been commercially available for a few years, and it is too early to predict much about its future. It should have good possibilities in new topnote creations for perfumes of the citrusy, herbaceous and mildly fruity character, while it does not seem to be very compatible with woody notes. It gives excellent support to Bitter Orange oil in topnote compositions.

The title aldehyde could possibly be used in flavors, since it has much of the "cooked" or even "baked" fruit note, e.g. baked Apple, Orange, etc. It is also buttery, Coconut-like in concentrations lower than 5 ppm, but rather violent and dominating at higher levels.

Prod.: from Croton aldehyde and *n*-Heptanal by condensation. Also by double addition of Acetaldehyde to Heptanal.

Sample: Compagnie Parento, USA.
See also monographs:
Decadienal (820) and Dodecadienal (1101).

## 3023: 2,3-UNDECADIONE

Acetyl pelargonyl.
Acetyl nonyryl.
Acetyl nonanoyl.

$CH_3—CO—CO(CH_2)_7CH_3$

$C_{11}H_{20}O_2 = 184.28$

Intensely yellow oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Powerful, sweet-creamy, warm odor with a Coconut-oily note in extreme dilution. The undiluted material has a rather repulsive, medicinal-sweet odor, similar to that of Diacetyl, although much weaker.

Sweet-creamy and Coconut-milky taste in concentrations below 10 ppm.

The title material, although with the general characteristics of the *1,3*-Diketones ("Quinone"-type odor) has a much softer aroma than its lower homologues. It is probably not used in perfumes, but it finds some use in flavors, mainly Butter imitation flavor. The concentration in finished products is as low as 1 to 3 ppm, although it can be slightly higher in baked goods.

It works very well with Nonanolide and other Coconut-materials, and with lower Lactones in Nut or Butterscotch type flavors, and it will benefit from the presence of discrete amounts of fruity notes.

Prod.: (several methods) e.g. from Methyl nonyl ketone via the Monoxime of the title Diketone.

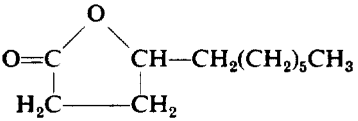
F.E.M.A. No.3090 – cleared by the American F.D.A. for use as a synthetic flavor substance.

66-721;

## 3024: gamma-UNDECALACTONE

Undecyllactone.
Undecanolide-*1,4*.
*1,4*-Hendecanolide.
"Aldehyde C-14, so-called".
*gamma-n*-Heptyl-*gamma*-butyrolactone.
"Peach Aldehyde".
"Persicol".
and many other trade names.

The commercial product consists mainly of the *gamma*-Lactone, while minute amounts of the desirable *delta*-Lactone are normally present.



$C_{11}H_{20}O_2 = 184.28$

Almost colorless or very pale straw-colored, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils, and in aqueous alkali.

Sweet, oily-fruity, Peach-like taste in concentrations lower than 20 ppm. The effect at higher concentrations is not unpleasant, but strongly fruity, supporting other fruity notes, necessarily present at high concentration of the Lactone.

This material is widely used, although in minute amounts, in perfume compositions. In order of frequency in use, it ranks very high among the materials on the perfumer's shelf. But it is not the kind of material ordinarily sold in drum-lots. However, after the success of a new perfume (type) in the 1950's, the title material had a further increase in popularity, when numerous perfumers used it at unusually high levels along with new non-Nitro musk chemicals, in order to duplicate part of the new note in the successful perfume. The author has yet to see a duplication which sells better than the original (in perfumes), but it must be admitted that Undecalactone drew benefit from this popularity.

It blends excellently with Nonalactone in Gardenia and Tuberose, and in many versions of Lilac bases. It extends the depth of an Orangeblossom often too harsh with conventional materials, and it is a frequent component of Honeysuckle, etc. Concentrations far below 1% are effective, and it is at times possible to ruin a fragrance with 0.1 or 0.2% of the title material, just as well as it is possible to double the floral sweetness and depth of another fragrance with that amount of Undecalactone.

The material was originally used in Violet perfumes, so popular at the time of discovery of this Lactone (about 1900). But its most important use today is in flavors, primarily in imitation Peach, but also in many fruity types, often as a fixative for the very volatile fruit esters.

Normal concentrations in finished products are 3 to 12 ppm, but it may be as high as 100 ppm in chewing gum. As mentioned above, the high concentrations demand considerable "construction" of heavy flavor chemicals around the Lactone, otherwise it will perform in a rather greasy-unpleasant manner. Vanillin, Palatone (Veltol), Ethyl Veltol, sweet Orange oil, etc. may support the Lactone and make it palatable at the high concentration and at the same time take advantage of the enormous effect in aroma volume increase supplied by this Lactone.

The name "Peach Aldehyde" is used stubbornly in the perfume industry, and it puzzles the chemist who knows that the material is not an aldehyde and does not have the disadvantages of an aldehyde in a composition. It is doubly amusing to notice the reports from the intense research on natural components of Peach pulp and juice. The Lactones with 6, 7, 8, 9, 10 and 12 Carbon atoms have been identified, while the Undecalactone – with 11 Carbons – has not been identified with certainty. Which makes the name "Peach Aldehyde" somewhat unjustly. However, one should not forget that the effect of the Lactone seems to please the customers, and that is generally what counts.

Prod.:

1) by Lactonization of Undecylenic acid with sulfuric acid. This process will yield minor amounts of *delta*-isomer.
2) from Octanol-*1* plus Methylacrylate, with Di-*tertiary*-Butylperoxide.
3) from Heptyl-ethylene oxide plus Sodiomalonic ester.

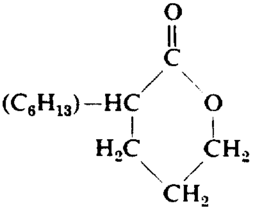
A number of other methods are known and used.

G.R.A.S. F.E.M.A. No.3091.

5-208; 31-172; 41-38; 90-666; 106-41; 156-230; 157-425; 163-75; 163-242; 163-381;
See also monographs:
*delta*-Undecalactone (3025).
*alpha*-Heptyl-*gamma*-butyrolactone (1523).
Other isomers of the title Lactone are known, but rarely used and almost never offered commercially.

## 3025: delta-**UNDECALACTONE**

*alpha-n*-Hexyl-*delta*-valerolactone.
Undecanolide-*1,5*.



$C_{11}H_{20}O_2 = 184.28$

Colorless, very viscous liquid. Sp.Gr. 0.96.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, creamy-fatty and in dilution pronounced Peach-like odor of excellent tenacity.

At concentrations below 10 ppm, the flavor is more typical Peach-like and less grassy than that of *gamma*-Undecalactone. The minimum perceptible is well below 0.1 ppm.

The author does not quite agree with literature stating that the *delta*-Lactones "lack the pleasant grassy notes of the *gamma*-Lactones". However, it is a very subjective matter, if the "grassy" notes are desirable or not.

The title Lactone has been developed for use in perfumes and flavors, and it has found use primarily in flavors for its pleasant "creamy" effect. This effect is of interest in Icecream with a multitude of flavor types, not only Vanilla and Peach, and in baked goods to enhance the mellowing flavor effect of Butter, further in various beverages as a mellowing flavor agent (fruit, cream-soda etc.). It is generally used in Milk, Butter and Peach imitation flavors, and the concentration in finished products is about

1 to 2 ppm in beverages,
2 to 5 ppm in Ice cream,
5 to 20 ppm in baked goods.

The material is highly interesting in Magnolia, Gardenia, Tuberose and other floral bases, and as a trace additive to Ylang Ylang in other perfume types.

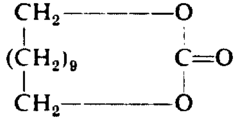
Prod.: from Heptaldehyde plus Acetaldehyde, via *3*-Nonenal by Michael's addition of Acetaldehyde to *2*-Hexylglutaraldehyde. Internal Canizzaro's reaction yields the cyclized Lactone.

31-175; 66-717; 66-801; 158-106; 159-420; 163-242;

Sample and data: Soda Aromatic Co., Ltd. Sept. 1967, Osaka, Japan.

## 3026: UNDECAMETHYLENE CARBONATE

Undecamethylene carboxylate.



$C_{12}H_{22}O_3 = 214.31$

Colorless oily liquid.

Insoluble in water, soluble in alcohol and oils.

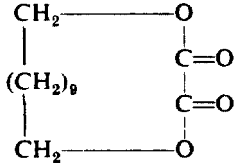
Musky, but not altogether sweet odor, faintly woody-camphoraceous notes of considerable tenacity.

The title material was developed in search of new "macrocyclic" musks, and has had little success. Apart from the academic interest in the study of these musks, it has no longer application in perfumery. It represents in a sense the "borderline" between acceptable musk odors, and uninteresting woody odors in the series of cyclic compounds of this structure. The higher homologues are more interesting and possible candidates for perfumery use, while the lower homologues are without interest to the perfumer.

Prod.: from Undecamethylene glycol with Butylcarbonate and Sodium, followed by depolymerization by heat.

31-127; 159-439;

## 3027: UNDECAMETHYLENE OXALATE



$C_{13}H_{22}O_4 = 242.32$

Opaque fused mass or colorless viscous liquid. M.P. 24° C.

Insoluble in water, soluble in alcohol and oils.

Powerful and sweet, very tenacious musky odor with little or no trace of animal note.

The title material could be of interest to the perfumer if the ester were made commercially available at a competive price. Competitive with the macrocyclic musks of similar odor – e.g. Ethylene brassylate, etc.

It is possible that the title material is used under trade name.

It represents one of a series of musks developed under French patent No.796410 in 1936 – before the Ethylene brassylate became known.

However, it seems that the title material cannot compete with the newer musks, and one may assume that it is practically obsolete in perfumery.

Prod.: from Undecamethylene glycol and Dibutyloxalate with Sodium, followed by depolymerization by heat.

31-128; 156-262; 159-440;

## 3028: UNDECANAL

Undecaldehyde.
Hendecanal.
*n*-Undecylic aldehyde.
*alpha*-Oxo-undecane.
Aldehyde C-11 (saturated).

$CH_3(CH_2)_9CHO$

$C_{11}H_{22}O = 170.30$

Colorless oily liquid. Sp.Gr. 0.83.
B.P. 223° C.

Solidifies in the cold, melts at 25° C.

Polymerizes under exposure to air.

Practically insoluble in water, soluble in alcohol and oils.

Pleasant waxy-floral, refreshing odor with a discrete fruity overtone and moderate tenacity. Very high grade material will fade out and leave no terminal notes, while impure material often show acid or overly fatty notes near the dryout on a blotter test.

Citrusy-fresh taste in concentrations below 10 ppm. Not pleasant at higher levels unless accompanied by a flavor composition.

This aldehyde – sometimes referred to as "Aldehyde C-11" – is used quite widely in perfume compositions, in very small proportions. The material seems to have fluctuating popularity, sometimes being used more frequently than the unsaturated Undecylenic aldehyde (see *10*-Undecenal), and then again being neglected in favor of the unsaturated aldehyde for another period. The two aldehydes are not interchangeable in a composition, but they do have certain effects in common. Special isomers of the unsaturated aldehyde have now been made commercially available and prove to be much more powerful than any of the conventional C-11 aldehydes.

Traces, usually less than 0.5%, are used in floral compositions, Rose, Tuberose, Cassie, Jasmin, etc. and in "incense" (Olibanum) compositions, "fresh-air" odors, Orris compositions, etc. as well as in topnote compositions of Citrus oils or fruity materials. It lends good support to Verbena.

Concentrations equal to 1 to 3 ppm in finished products are used in imitation Lemon, Lime, Mandarin, Orange, Cucumber, Honey and various fruit complexes, for waxy-honey-like notes, fresh notes, etc. Concentrations in chewing gum may be as high as 50 or 60 ppm.

G.R.A.S. F.E.M.A. No.3092.

Prod.: (many methods) e.g. from Coconut oil via Lauric acid, Lauryl chloride, Laurylbromochloride, and by the hydroxyacid to the title aldehyde. Or from Castor oil via Undecylenic acid to its ester and the title aldehyde.

5-83; 31-49; 41-33; 31-57; 89-31; 106-37; 128-289; 140-159; 156-19; 163-74; 163-243; B-I-712;

## 3029: UNDECANAL DIETHYLACETAL

Aldehyde C-11, diethylacetal.
Undecylaldehyde diethylacetal.

$CH_3(CH_2)_9CH(OC_2H_5)_2$

$C_{15}H_{32}O_2 = 244.42$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Soft, oily-citrusy odor of moderate to good tenacity.

The title acetal has not had much success in perfumery, and it seems that most perfumers do not even have the material on the shelf. It is rarely offered commercially, and it could be partly because of old and stubborn belief, that the acetals are "just weak versions of the aldehydes". It is not always so. Far from.

It is true that this acetal is much milder than the parent aldehyde, but it has an entirely different odor type, and different suggested application. In fact, it would offer an excellent "liaison" between the topnote and the main theme of a fragrance. It could form part of the classical method of a "fixation gradée" after the topnote.

Its mildly oily-winey character makes it particularly suitable for Rose and other florals, but it is also useful in Citrus colognes, and blends well with Labdanum.

Prod.: by condensation of Undecanal and Ethylalcohol.

163-74;

## 3030: UNDECANAL DIMETHYLACETAL

Undecylic aldehyde dimethylacetal.
*omega-omega*-Dimethoxy undecane.
Aldehyde C-11, DMA.

$CH_3(CH_2)_9CH(OCH_3)_2$

$C_{13}H_{28}O_2 = 216.37$

Colorless liquid.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, oily-floral, citrusy odor with mildly herbaceous-green notes and moderate tenacity.

This acetal is occasionally used in perfume compositions as a modifier for the aldehyde, mellowing and extending its effect into a wider field, beyond the topnote, where the aldehyde almost inevitably works.

The acetal is rarely offered commercially, and it is absent from most perfume laboratories. Among those who favor the use of this material, there are many perfumers who find it superior to the Dimethylacetal of the unsaturated aldehyde (Undecenal dimethylacetal).

The title material is particularly interesting in Citrus compositions, fresh-herbaceous fragrances, Lavender-Fougères, and mild floral Rose or Muguet bases.

Prod.: from Undecanal and Methanol, usually with dry hydrogen chloride as condensing agent, or with Ferrichloride or similar catalyst.

## 3031: UNDECANOL-1

Undecyl alcohol.
Undecylic alcohol.
Alcohol C-11 (saturated).
Decyl carbinol.
*l*-Hendecanol.

$CH_3(CH_2)_9CH_2OH$

$C_{11}H_{24}O = 172.31$

Colorless oily liquid, solidifying in the cold.
M.P. 16°C. Sp.Gr. 0.83. B.P. 241° C.

Almost insoluble in water, soluble in alcohol and oils.

Oily-fruity, floral-citrusy odor, slightly fatty, but overall fresh and delicately rosy, in high dilution Mandarin-like.

Concentrations below 20 ppm have citrusy, oily-fruity, mildly sweet taste, but higher concentrations tend to produce unpleasantly fatty taste.

This alcohol is frequently, but not very widely used in perfume compositions, often as a companion to the corresponding aldehyde or other alifatic aldehydes in topnote compositions, etc. It blends well with the floral-citrusy fragrance types, Citrus colognes, Cassie and Violet, green and herbaceous fragrances, etc. It is often used in Rose bases.

In imitation Citrus flavors, Lemon, Lime, Mandarin and Orange, and occasionally in Blackcurrant flavor or Rose flavor, it is used in small amounts, equivalent to 3 to 15 ppm in the finished product.

G.R.A.S. F.E.M.A. No.3097.

Prod.:

1) by Bouveault-Blanc reduction of Ethyl undecylate.
2) by reduction of Ethyl undecylenate.
3) by Grignard reaction from *n*-Nonyl magnesiumbromide plus Ethylene oxide.

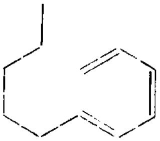
36-819; 41-25; 106-30; 128-288; 140-125; 156-13; 163-74; 163-243; B-I-427;
Undecanol-*2* is mentioned under the title: Methyl nonyl carbinol.

## 3032: UNDECATRIENE-1,3,5

Undeca-*1*,*3*,*5*-triene.

$CH_2{=}CH{-}CH{=}CH{-}CH{=}CH{-}CH_2{-}CH_2{-}CH_2{-}CH_2{-}CH_3$

or:



$C_{11}H_{18} = 150.27$

Colorless mobile oil.

Insoluble in water, soluble in alcohol and oils. Polymerizes in air and becomes yellowish or darker, more viscous, less odorous.

Powerful, gassy-green and very diffusive, but in dilution pleasantly oily-herbaceous, vegetable-green, warm odor of moderate to poor tenacity.

The title triolefin was synthesized a few years ago after an intensified research aimed at the odorous components in Galbanum. Of the non-terpeny components, the title material proved to be one of the more interesting and apparently important to the odor picture of Galbanum. The natural material had a temporary uptrend in market price, culminating in 1964 with a cost almost 10 times the normal. This initiated the research, otherwise neglected. But when the natural material is very important in a successful perfume, or if the material is used in multi-ton lots annually by one perfume house, such price fluctuations become critical.

It is interesting to notice further, that Myrcene and Ocimene, both triolefins, are also present in Galbanum (volatile part). They are branched-chain, lower homologues of the title material, but may not be derived from that, nor be intermediates of the title material.

If the title hydrocarbon becomes freely available, it will undoubtedly find use in revised versions of several successful perfumes. Countless "copies" were developed as soon as it was revealed that "Miss Dior" contained Galbanum products as one of the key components, and within a few years every other "luxury" perfume contained Galbanum, hoping to get a share of the success. The story speaks for itself about lack of "originality" in modern creative perfumery, or it may prove that Galbanum is not the only key to success.

Prod.: One synthesis is based upon dehydration of Undeca-*1*,*5*-dien-*3*-ol.

## 3033: 2-UNDECEN-1-AL

Undecen-*2*-al.
*3*-Octyl acrolein.
*trans*-*2*-Undecenal.
Sometimes called: 9-Undecenal – see NOTE below.

$CH_3(CH_2)_7CH{=}CH{-}CHO$

$C_{11}H_{20}O = 168.28$

Colorless or very pale straw-colored oily liquid. Sp.Gr. 0.86. B.P. 229° C.

Insoluble in water, soluble in alcohol and oils.

Powerful, in dilution very refreshing, sweet-citrusy, Orange-peel like odor, diffusive and yet quite tenacious. The undiluted material is rather overwhelming in its odor intensity, difficult to appreciate.

Sweet citrus-like taste in dilutions near 1 ppm, but the taste is vastly improved in the presence of food acids.

This aldehyde is a member of a relatively large family of *3*-Alkyl substituted Acroleins, of which the lower members are probably the best known and most widely used in perfumes and flavors.

The title unsaturated aldehyde is relatively new on the market but has already found application in perfumes for its great power and pleasant effect at proper (very low) level of concentration. It gives interesting effects with the conventional alifatic aldehydes in Citrus topnotes, and it goes much further, deep into the heart of the fragrance, where for instance, Undecanal would not reach.

As a novel note in Oriental fragrance bases, it blends very well with Opopanax, Rose, Neroli, etc. and it is also interesting in modern fragrances for men with Clary Sage, Lavender, Hay-notes and various "fresh-outdoor" materials, such as Mentha Citrata No.664 (Todd Co.), Coriander, Moroccan Chamomile, etc.

Although the material is not yet included in the American G.R.A.S. list of food flavor materials, it could be used experimentally in the creation of new and highly interesting Citrus imitation flavors. It gives very pleasant effect and great power in Butterscotch, where conventionally the terpeneless type Orange oil is often used. It is conceivable that the material can eventually be approved for food flavors, and it may therefore serve a purpose to make the experiments meanwhile.

Prod.: by condensation of Acetaldehyde with Nonanal. It can also be produced via *alpha*-Bromo undecanoic acid.

163-242; 156-26;
Sample: Compagnie Parento, Inc., USA.
NOTE: *9*-Undecen-*1*-al and *10*-Undecen-*1*-al (see later monographs) are both specifically included in the American G.R.A.S. list and the author suspects that the perfume and flavor industry has brought about some confusion between the "*9*-Undecenal" and the title aldehyde.

## 3034: 9-UNDECENAL

Hendecen-*9*-al.
Undecylenic aldehyde (an isomer).
The structure of the title material could be:

$$CH_3{-}CH{=}CH(CH_2)_7CHO$$

$$C_{11}H_{20}O = 168.28$$

and the correct chemical name of this material would be:

*9*-UNDECEN-*1*-AL

The title material is included in this work because it is mentioned in food literature and specifically included in the American G.R.A.S. list – as different from *10*-Undecen-*1*-al (see nonograph).

The author suspects a confusion with *2*-Undecen-*1*-al, although the odor description published for the title aldehyde ("much weaker than the odor of *10*-Undecen-*1*-al") does not agree with the author's impression of the odors. *2*-Undecen-*1*-al has a much more powerful and much sweeter odor than that of *10*-Undecen-*1*-al.

The title aldehyde has been suggested for use in Citrus and Nut flavor compositions, and that use is in agreement with the suggested use of *2*-Undecen-*1*-al.

G.R.A.S. F.E.M.A. No.3094.
See also monographs:
*2*-Undecen-*1*-al.
*10*-Undecen-*1*-al, and
Undecenal (mixed isomers).

## 3035: 10-UNDECEN-1-AL

*n*-Undecenoic aldehyde.
Undecylenic aldehyde.
Hendecen-*10*-al.
Aldehyde C-11, unsaturated.
Many specialties are based wholly or partly upon this aldehyde:
"Pekleol" (de Laire).
"Ambrolione" (Firmenich), etc.

The commercial product consists almost entirely of the so-called "terminal" isomer, in which the point of unsaturation is opposite of the Aldehyde group. Aldehyde with unsaturation in position "8" may form a minor by-component.

See also monograph: Undecenal (mixed isomers), next.

$CH_2{=}CH(CH_2)_8CHO$

$C_{11}H_{20}O = 168.28$

Colorless liquid. Solidifies in the cold.
M.P. 7° C. Sp.Gr. 0.84. B.P. 235° C.

Practically insoluble in water, soluble in alcohol and oils.

Powerful, mildly waxy, rosy-citrusy odor of moderate to good tenacity. The odor could be classified as one of the prototypes of the term: "aldehydic" odor.

Concentrations below 1 ppm have pleasant, refreshing fruity-citrusy taste, preferably in presence of food acid.

The material polymerizes in air, and forms adduct (addition-products) with Amines (Indole, Anthranilates, Quinolines, etc.).

The title aldehyde is one of the most frequently used of all the alifatic aldehydes, although the concentration in perfume oils is normally as low as 0.1 to 0.5%. Its unusual diffusive power, the lift and radiation it can introduce in a fragrance, are highly appreciated effects even in soap perfumes. As a supporting note to Rose, Ambre, Moss and many other fragrance types, it is a very versatile material.

Its chemical Nature was more thoroughly investigated in the early 1960's and results from such investigations include the commercial availability of specific isomers, some of which have exceptional power and fragrance beauty (see Undecenal, mixed isomers). But the title material remains as one of the most popular "aldehyde notes" in modern perfumery, including very common use, due to the power and relatively low cost of this material.

The aldehyde is used in minute traces – about 0.1 to 0.3 ppm in finished products – for imitation Citrus flavors, and in various fruity and floral flavor types. The *2*-Undecen-*1*-al is undoubtedly more interesting for flavor purposes.

Prod.:
1) by catalytic oxidation of *10*-Undecen-*1*-ol (see monograph).
2) from Undecylenic acid and Formic acid under heat and pressure.

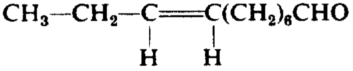
Many other methods are in use.
G.R.A.S. F.E.M.A. No.3095.

5-88; 106-36; 128-290; 156-23; 163-74; 36-915;

## 3036: UNDECENAL (mixed isomers)

Undecylenic aldehyde, "internal isomers".
"Intreleven Aldehyde" (I. F. & F.).

The commercial product under the trade name "Intreleven Aldehyde" is a mixture of several isomers of Undecylenic aldehyde, with emphasis upon the *cis-8*-Undecen-*1*-al:

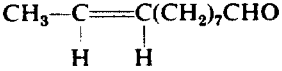


$CH_3{-}CH_2{-}\underset{H}{C}{=}\underset{H}{C}(CH_2)_6CHO$

= *cis-8*-Undecen-*1*-al,

$C_{11}H_{20}O = 168.28$

also with some



$CH_3{-}\underset{H}{C}{=}\underset{H}{C}(CH_2)_7CHO$

= *cis-9*-Undecen-*1*-al,

and variable amounts of the "terminal" isomer (see previous monograph) plus other isomers.

Colorless liquid. Practically insoluble in water, soluble in alcohol and oils.

Very powerful and diffusive, refreshingly citrusy-waxy, in extreme dilution dry-floral, "clean" odor.

The radiance of this material is its greatest asset, but it is also, in the opinion of most perfumers, superior in odor type, over the regular Undecylenic aldehyde. The "clean" odor could also be described in that the odor of the title aldehyde is less "fatty" than that of the regular grade. The citrusy character is nearest to Orange in suitable dilution.

This material was brought into commercial production when it was discovered that Undecylenic aldehyde "was not always just Undecylenic aldehyde". There were materials of entirely different strength - from different manufacturers. As a compromise between reasonable cost and practical synthesis, the title material was marketed, with a certain amount of the particularly desirable and highly powerful isomers in a base of regular aldehyde.

Although the manufacturer claims that the material is about five times stronger than regular Undecylenic aldehyde, one should not assume that this is a substitute for "old-fashioned" Undecylenic aldehyde. It does have a different odor, cleaner and fresher, and its effect is probably from two to four times stronger, if it can be compared at all to the regular aldehyde. The cost is also about three times that of the regular aldehyde.

The title aldehyde (mixture) performs beautifully in soap, and since it can be applied at a fraction of one percent, its relatively high cost does not really limit its use. It gives excellent support to Rose, but it is particularly interesting for "new" experiments in creative perfumery, Ambre, Moss, fruity and "fresh-air" notes, e.g. with the Mentha Citrata Todd oil No.664, and with many new Ambregris materials, Lime materials, etc.

Prod.:

1) by isomerization of Undecylenic aldehyde ("regular").
2) by catalytic oxidation of isomerized Undecylenic alcohol.

Certain isomers monitor the strength and beauty of this mixture, and the final product must be composed partly by chemical specifications.

Material: I.F. & F. Inc. (USA).

## 3037: UNDECENAL DIETHYLACETAL

Aldehyde C-11, diethylacetal.
Undecylenic aldehyde (regular), diethyl acetal.

$CH_2{=}CH(CH_2)_8CH(OC_2H_5)_2$

$C_{15}H_{30}O_2 = 242.41$

Colorless oily liquid.

Almost insoluble in water, soluble in alcohol and oils.

Very soft, oily-citrusy, and in extreme dilution mildly citrusy-fruity, and Brandy-like, sweet odor.

This acetal is occasionally offered commercially, but it seems to have failed its attempts to catch any interest from the perfumers. It simply does not offer any unusual notes or exceptional stability when compared to the aldehyde or other conventional materials covering its odor characteristics.

Undecylenic aldehyde performs very well in soap, and the acetal has nothing special to offer here, except that it is definitely weaker, and not interchangeable with the Aldehyde.

The acetal could possibly find use in flavors, as a modifier in Citrus and Brandy (imitation) compositions.

Prod.: by condensation of Undecenal (regular type) with Ethyl alcohol.

163-74;

## 3038: 2-UNDECEN-1-OL

*3*-*n*-Octyl-*2*-propen-*1*-ol.

$CH_3(CH_2)_7CH{=}CH{-}CH_2OH$

$C_{11}H_{22}O = 170.30$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Very powerful, sweet-oily, in dilution floral, rosy, softly waxy odor of moderate tenacity.

This alcohol, the aldehyde of which is also known and used, has only recently become commercially available, although still scarce and rare in the perfume laboratories.

It offers new variations in the diffusive rosy and citrusy fragrances and is overall an interesting material for experiments in novel creations. It performs very well with Bergamot and the new Mentha Citrata (Todd) No.664 oils, and with the alifatic aldehydes in topnote compositions, where it may extend the "lifting" effect further into the heart of the fragrance.

Prod.: (several methods) e.g. from Acrolein and Octyl magnesium chloride to yield *n*-Octyl vinyl carbinol. Anionotropic rearrangement with Phosphorus tribromide, followed by treatment with Potassium acetate and hydrolysis then yields the title unsaturated alcohol.

66-315; 163-243;

## 3039: 10-UNDECEN-1-OL

Undecen-*1*-ol-*11*. See NOTE below.
Undecenyl alcohol.
Undecen-*10*-ol-*1*.
Undecylenic alcohol.
Alcohol C-11 (unsaturated).
*n*-Undecenoic alcohol.

As seen from the above synonyms, the commercial literature gives ample room for confusion in the nomenclature.

$CH_2{=}CH{-}(CH_2)_8CH_2OH$

$C_{11}H_{22}O = 170.30$

Colorless oily liquid. Sp.Gr. 0.85.
B.P. 245° C.

Almost insoluble in water, soluble in alcohol and oils.

Fresh, but rather fatty odor (variable amount of fatty notes in different grades of this alcohol) with citrusy-waxy and rosy, petal-like notes.

Concentrations below 5 ppm have pleasant, fresh-citrusy, slightly floral taste. Higher concentrations tend to appear overly fatty.

The title alcohol finds some use in perfume compositions, mainly to give "lift" to Rose, Jasmin, Magnolia, Violet, Lilac, Cassie and other floral fragrances, and in Citrus topnotes or fruity notes. It is somewhat more versatile than the corresponding aldehyde.

Traces are also used in Citrus imitation flavors and in floral flavor types.

Prod.: by various methods, usually starting from Undecylenic acid, which is obtained from Castor oil.

Cleared for use in food products by the American F.D.A.

36-816; 41-26; 106-29; 156-15; 163-74; B-I-452;

NOTE: Some producers claim that their product is *9*-Undecen-*1*-ol. The author has not been able to confirm such statement. The listing of the acetate of the title alcohol as "*9*-Undecen-*1*-yl acetate" in the Publication 1274 from the American Academy of Sciences, National Research Council (USA) may also be an error.

## **3040: UNDECENOL** (mixed isomers)

$C_{11}H_{22}O = 170.30$

The title material is a mixture of alcohols, corresponding to the mixture of aldehydes listed under the monograph:
UNDECENAL (mixed isomers).

This material, rarely available under its chemical name, has been suggested for use in perfume compositions. However, it has not attracted nearly the same amount of attention as given to the aldehyde-product.

One of the isomers, not with certainty identified in the above product, has been identified in Nature: *1*-Undecen-*10*-ol, also called Hendecen-*10*-ol-*2*.

Apart from experimental use in new top-note compositions, the title material has found very little use in perfumery.

Prod.: by isomerization of Undecylenic alcohol (regular, "terminal"isomer).

87-490; see also monograph: Undecenal (mixed isomers).

## **3041: UNDECENYL ACETATE**

Undecylenic acetate.
Acetate C-11 (unsaturated).
*10*-Hendecenyl acetate.
*10*-Undecen-*1*-yl acetate.
See NOTE under monograph: *10*-Undecen-*1*-ol.

$CH_2{=}CH(CH_2)_9{-}OOC{-}CH_3$

$C_{13}H_{24}O_2 = 212.34$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 272° C.

Practically insoluble in water, soluble in alcohol and oils.

Mildly fruity, fatty-floral, Honey-Rose type odor of good tenacity. Variations in this odor picture are observed in products from different suppliers.

Concentrations below 20 ppm have refreshingly fruity-citrusy taste, but this impression is not truly pleasant without a food acid.

The title ester finds a little use – one should say: too little use – in perfumery. It gives very pleasant and interesting effects in floral as well as non-floral (Ambre-Chypre, fruit, etc.) fragrance types, and it is exceptionally stable. Experiments in powder perfumes confirm this. As a refreshing note in Rose, Muguet or Lily, it adds valuable notes to otherwise dull perfumes in face powders, where freshness is a very rare virtue of the fragrance.

The ester is also used in trace amounts in fruit and Citrus imitation flavor compositions. The concentration in finished products may be about 3 to 15 ppm.

G.R.A.S. F.E.M.A. No.3096.

Prod.: by azeotropic type esterification of *10*-Undecen-*1*-ol with Acetic acid.

35-854; 41-17; 43-504; 106-20; 163-75; 163-382;
See also NOTE under: *10*-Undecen-*1*-ol.

## **3042: UNDECENYL**-iso-**BUTYRATE**

*10*-Undecen-*1*-yl-*iso*-butyrate.
*omega*-Undecenyl-*iso*-butyrate.

$CH_2{=}CH(CH_2)_9{-}OOC{-}CH(CH_3)_2$

$C_{15}H_{28}O_2 = 240.39$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 288° C.

Practically insoluble in water, soluble in alcohol and oils.

Relatively powerful, oily-fruity, rather heavy odor of considerable tenacity. The fruity notes tend to appear winey, Plum-like, depending upon the concentration.

This ester is very rarely offered commercially, but occasionally manufactured by an interested user. It may serve as a modifier in fruity-floral fragrance complexes, Gardenia, Tuberose, etc., where heavy-oily notes are sometimes desirable.

The author has no report of its use in flavor compositions.

Prod.: by azeotropic type esterification of *10*-Undecen-*1*-ol with *iso*-Butyric acid.

163-75; see also monograph: *10*-Undecen-*1*-ol (NOTE).

## 3043: UNDECENYL FORMATE

*10*-Undecen-*1*-yl formate.
*omega*-Undecenyl formate.

$CH_2{=}CH(CH_2)_9{-}OOCH$

$C_{12}H_{22}O_2 = 198.31$

Colorless oily liquid. Sp.Gr. 0.85.
B.P. 265° C.

Practically insoluble in water, soluble in alcohol and oils.

Peculiar, dry-sweet, very rich, unripe-fruity odor of good tenacity. The author has been unable to undersign odor descriptions including terms such as "fermented Honey", "acetous odor", "sharp", etc. but it is quite conceivable that such notes may appear in decomposed ester.

The title material has been suggested for use in perfume compositions, but it does not seem to have gained much ground in the perfume laboratory. If initial samples have been partly deteriorated, or were soon decomposing in the sample bottle, an evaluation of the material would of course not be in favor of any future use of it. This is most unfortunate and often occurs with Formates, particularly if they are not absolutely free from acid and moisture in the first place.

However, the perfume industry would not suffer any great loss to be without this item.

Prod.: by cold Formylation of *10*-Undecen-*1*-ol.

35-854; 103-87; 163-75;
See also NOTE under: *10*-Undecen-*1*-ol.

## 3044: UNDECENYL HEPTOATE

*10*-Undecen-*1*-yl heptanoate.
*omega*-Undecenyl heptylate.

$CH_2{=}CH(CH_2)_9{-}OOC{-}C_6H_{13}$

$C_{18}H_{34}O_2 = 282.47$

Colorless oily liquid. Sp. Gr. 0.88.
B.P. over 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Very faint, oily-winey odor of considerable tenacity. Upon intense study, one may observe a delicate greenness which is much more perceptible once the material is composed with more volatile materials.

This ester was probably developed in an attempt to find a typically "oily" odor of good tenacity. The oily greenness from the Heptanoic acid radicle and the mild, oily floralness from the Undecylenic portion should merge into a – hopefully – ideal combination product. But the product is not so ideal. In fact, it is not very interesting at all, except perhaps for academic studies.

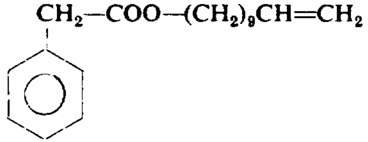
The material is very rarely offered commercially, and rarely found in the perfume laboratory.

Prod.: by azeotropic type esterification of *10*-Undecen-*1*-ol with *n*-Heptanoic acid.

163-75;
See also NOTE in monograph: *10*-Undecen-*1*-ol.

## 3045: UNDECENYL PHENYLACETATE

*10*-Undecen-*1*-yl-*alpha*-toluate.
*omega*-Undecenyl phenylacetate.



$C_{19}H_{28}O_2 = 288.43$

Colorless viscous liquid, solidifying in the cold. B.P. over 300° C.

Insoluble in water, soluble in alcohol and oils.

Very faint, but very tenacious, sweet, fruity-musky odor. Samples of different origin show considerable difference in odor, some have a very dominating "Phenylacetic" note, which is generally not desirable.

The title ester was probably developed by routine in search of new Phenylacetates with potential interest to the perfumer. The very high boiling esters have always intrigued certain groups of perfumers and perfume chemists, but the physical virtues of these materials are not always accompanied by similar olfactory excellence.

In brief, the material is of little interest, and may be practically obsolete already.

Prod.: from Phenylacetyl chloride and *10*-Undecen-*1*-ol.

The "metameric" ester, Phenylethyl undecylenate is somewhat more interesting, although of very limited use in perfumery. See monograph No. 2556.

163-75;
See also NOTE under monograph: *10*-Undecen-*1*-ol.

## 3046: UNDECENYL PROPIONATE

*10*-Undecen-*1*-yl propanoate.
*omega*-Undecenyl propionate.
Undecylenyl propionate.

$CH_2{=}CH(CH_2)_9{-}OOC{-}C_2H_5$

$C_{14}H_{26}O_2 = 226.36$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 282° C.

Practically insoluble in water, soluble in alcohol and oils.

Oily-fruity, mildly winey-fruity and very tenacious odor. The overall impression is that of a fruity, more than a floral type, although in suitable composition, the material is very compatible with Rose notes.

Not very often found in price lists, this material has been suggested for use in perfumes, mainly as a modifier for the acetate, where more fruity and less floral effect was acceptable. However, the ester does not really contribute much to a fragrance, and considering its cost which is far above average for fruity-floral esters to be used at medium-high concentration levels, there is not much speaking in favor of this material, except for occasional use in face powder perfumes.

It could find some use in Brandy, Rum, Citrus and similar flavor creations on account of its excellent stability which makes it suitable for flavors intended for baked goods etc.

Prod.: by azeotropic type esterification of *10*-Undecen-*1*-ol with Propionic acid.

163-75;
See also NOTE under monograph: *10*-Undecen-*1*-ol.

## 3047: UNDECYL ACETATE

Undecanoic acetate.
See NOTE below.

$CH_3(CH_2)_{10}{-}OOC{-}CH_3$

$C_{13}H_{26}O_2 = 214.35$

Colorless oily liquid. Sp.Gr. 0.86.
B.P. 268° C.

Practically insoluble in water, soluble in alcohol and oils.

Mild, oily-ethereal, soft-fatty, rosy odor of considerable tenacity.

This ester is used in amounts of a few percent as refreshing note in topnotes, mainly for Rose and Citrus type fragrances. The quality of the ester is very important, since traces of the parent components from the manufacture can ruin the delicately mild odor of this ester.

NOTE: Considerable confusion is derived from the fact that the acetate of the secondary Undecyl alcohol has been offered under the name Undecyl acetate. The correct name for the material is Methyl nonyl carbinyl acetate, or *secondary*-Undecylacetate (Undecan-*2*-ol acetate).

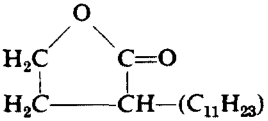
That material is included under its proper name in this work. It is sometimes described as having a green-herbal, incense-like note apart from its oily fatty odor, to a certain degree related to that of the title material.

Prod.: by direct esterification under azeotropic conditions with *n*-Undecanol and Acetic acid.

35-854; 43-504; 103-100; 163-382;

## 3048: alpha-n-**UNDECYL**-gamma-**BUTYROLACTONE**

A Pentadecanolide, not to be confused with Cyclopentadecanolide, a macrocyclic (isomer) musk.



$C_{15}H_{28}O_2 = 240.39$

Colorless, very viscous liquid, solidifying in the cold.

Practically insoluble in water, soluble in alcohol and oils.

Sweet, fatty-musky odor with variable amounts of fruity or Coconut-type oily-fatty, but pleasant notes of very considerable tenacity.

This material could, at first glance (with the nose) appear to be a good candidate for a generally applicable perfume musk. It is, however, not inexpensive in preparation, and its synthesis includes difficulties with undesirable isomers, etc. In other words, it is not very practical from a production point of view. And since its odor type is not among the most desirable and highly appreciated ones, there is only some academic interest in this material.

It is an empirical isomer of Cyclopentadecanolide, one of the truly unsurpassed musks, but it does not come near this idol in performance or exalting effect. To the student of olfactory behavior of odorous chemicals, this material is interesting because it is not a "macrocyclic" musk, while it has the empirical formula of the finest musk of all.

Prod.: from Undecyl malonic ester and Ethylene oxide. Other methods have been suggested with little economic improvement.

The isomer, Decyl valerolactone, is said to be odorless. The unsaturated lactone Undecenyl butyrolactone, is also known.

31-170; 156-229; 159-418; 159-420; 159-421; 163-243; 163-382;

## 3049: UNDECYLENIC ACID

Hendecen-*1*-oic acid-*11*.
*10*-Hendecenoic acid.
*10*-Undecenoic acid.
*9*-Undecene-*1*-carboxylic acid. (This name is often a source of confusion).

$CH_2{=}CH(CH_2)_8COOH$

$C_{11}H_{20}O_2 = 184.28$

Colorless leafy crystals or fused mass.
M.P. 24-25° C. B.P. 279° C. under decomposition. Sp.Gr. 0.91 (liquid).

Practically insoluble in water, soluble in alcohol and oils.

The odor varies enormously in different grades of the acid, from oily, mildly acid and heavy-fruity, overall pleasant, to acrid-acrid, repulsively sour-fatty. However, for perfumery or flavor purposes, the latter type would be absolutely out of question. The author therefore cannot agree with common descriptions of the odor as "sweat-like, unpleasant, etc.". This quality is unsuitable for perfumes, and also for many chemicals to be processed from the acid (see below).

A very highly refined grade of this acid has a faintly Peach-like odor, accompanied by a waxy-fatty, mildly sour-sweet note which gives an overall pleasant impression. It is true, however, that the "normal" grade, which is an industrial chemical, produced in volume of thousands of tons, sold in railroad tank cars, has a much inferior color, odor and general appearance.

The acid is rarely used as such in perfumes or flavors, except perhaps in certain artificial flower absolutes, etc. and for very special odor effects.

It represents one of the two chemicals, obtained directly from Castor oil, making Castor oil one of the most important natural raw materials for the manufacture of perfume and flavor chemicals. The other chemical from Castor oil is Heptaldehyde (see monograph).

Undecylenic acid is reduced to Undecylic acid, and it can be oxidized to Sebacic acid. It is a starting material for the manufacture of Undecanolide, Undecylenic aldehyde, many new "non-Nitro" types of musk, esters, alcohols, ketones, etc.

Prod.: Mostly by thermal decomposition (pyrolysis under vacuum) of Castor oil (or Methyl ricinoleate).

It has also been synthesized by the Malonic ester method.

The 9-Undecenoic acid is also industrially known.

1-210; 66-638; 90-122; 100-1079; B-II-458;

## 3050: UNDECYL FORMATE

Undecanoic formate.

$CH_3(CH_2)_{10}—OOCH$

$C_{12}H_{24}O_2 = 200.34$

See also comments under Undecyl acetate, about the isomer of the ester.

Colorless liquid. Sp.Gr. 0.86. B.P. 263° C.

Dry-oily, mildly herbal or discretely green odor, reminiscent of certain dried herbs, without being "aromatic".

The title ester finds a little – probably very little – use in perfume compositions, mainly as part of topnote compositions in herbaceous fragrance types, Lavender, Fougeres, and in variations of Rose, Magnolia, etc. It is also quite interesting as supporting note to Mandarin, a very favored topnote item, but unfortunately very unstable.

Prod.: by cold formylation of Undecanol.

35-854; 103-87;

## 3051: UNDECYLIC ACID

Undecanoic acid.
Decane-*alpha*-carboxylic acid.

$CH_3(CH_2)_9COOH$

$C_{11}H_{22}O_2 = 186.30$

Colorless crystals or crystalline mass.
M.P. 29° C. B.P. 284° C. Sp.Gr. 0.89 (liquid).

Almost insoluble in water, soluble in alcohol and oils.

Very weak, fatty-aldehydic odor with considerable variations according to origin (and purity). A high-grade material has practically no odor, while a normal commercial grade smells oily-fatty in a mild, sweet and not unpleasant manner, and with good tenacity.

The title saturated alifatic acid is only very rarely used as such in perfumes or flavors, but it is briefly mentioned in this work in connection with the unsaturated acid, Undecylenic acid, which is one of the most important chemical intermediates of this type.

Undecylic acid could be used in discrete amounts to support Costus notes and various musky notes, but the material does not contribute much to a fragrance as such. It is relatively unimportant in Nature and not widely distributed in plants.

It serves as a raw material for the manufacture of a number of esters, some of which are used in perfumes, more in flavor compositions.

Prod.: by reduction of Undecylenic acid, which is generally obtained from Castor oil. See monograph: Undecylenic acid.

1-194; 36-697; 66-564; 66-577; 90-97;
B-II-358;

## 3052: n-VALERALDEHYDE

*n*-Pentanal.
*n*-Valeric aldehyde.
Valeral.
Amylaldehyde.

$CH_3(CH_2)_3CHO$

$C_5H_{10}O = 86.14$

Colorless liquid. B.P. 103° C. Sp.Gr. 0.81.

Very slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Very powerful and diffusive, penetrating, acrid-pungent odor, in the concentrated form repulsively choking, cough-provoking. In extreme dilution dry-fruity, musty, Nut-like.

The taste of this material is best evaluated at concentrations below 10 ppm, where pungency, acid notes and choking vapors are not interfering. At this low level, the taste is warm, slightly fruity, herbaceous-Nut-like.

The title material is probably not used in perfumes. It is preferably removed from Eucalyptus oil by rectification (or by isolation of the useful Eucalyptol) prior to use in flavors, because the aldehyde would act cough-provoking, and this would be rather embarrassing since the Eucalyptus oil is often used in cough drops, etc.

Concentrations equal to about 1 to 5 ppm in finished products are used in imitation Nut and various fruit flavors, occasionally in Coffee, Caramel, etc.

G.R.A.S. F.E.M.A. No.3098.

Prod.: by reduction of *n*-Valeric acid.

36-1029; 66-477; 89-15; B-I-676;

## 3053: iso-VALERALDEHYDE

*2*-Methyl-*n*-butyraldehyde.
*iso*-Pentanal.
*3,3*-Dimethylpropanal.
*2*-Methylbutanal-*4*.
*iso*-Pentaldehyde.
*3*-Methylbutanal-*1*.
*iso*-Valeral.
*iso*-Amylaldehyde.

NOTE: An important isomer is listed in this work under:
*alpha*-Methyl butyraldehyde(=*2*-Methylbutanal-*1*).

$(CH_3)_2CH{-}CH_2{-}CHO$

$C_5H_{10}O = 86.14$

Colorless mobile liquid. Sp.Gr. 0.80.
B.P. 93° C.

Slightly soluble in water, soluble in alcohol, Propylene glycol and oils.

Very powerful, penetrating, acrid-pungent odor, causing cough-reflexes unless highly diluted.

In extreme dilution, the odor becomes fruity, rather pleasant, and the flavor is Peach-like, heavy-fruity below 10 ppm.

The title material is probably not used in perfumes.

It finds considerable use in flavor compositions, mainly for imitation Butter, Chocolate, Cocoa, Nut, Coffee, Caramel, etc. and in many fruit complexes. The concentration in finished products will be as low as 0.5 ppm up to 4 or 5 ppm.

The aldehyde is very reactive, and will form acetals with many flavor solvents, including Propylene glycol. The glycol-acetals in particular have entirely different organoleptic characteristics. However, the slightly acid conditions prevailing in most flavored products will normally discourage acetal-formation.

G.R.A.S. F.E.M.A. No.2692.

Prod.: (many methods) e.g. by reduction of *iso*-Valeric acid.

66-477; 36-1029; 89-16; B-I-684;

## 3054: VALERALDEHYDE DIAMYLACETAL

Diamylvaleral.
Dipentoxy pentane.

$CH_3(CH_2)_3CH(O—C_5H_{11})_2$

$C_{15}H_{32}O_2 = 244.42$

Colorless oily liquid.

Very slightly soluble in water, soluble in alcohol and oils.

Warm-spicy, ethereal-herbaceous odor with resemblance to Celery.

The title acetal has been suggested for use in perfume compositions, and it could possibly find use also in flavors.

A number of acetals from Valeric aldehyde have been prepared, but none more interesting than those made with the Glycols. These materials are rarely offered commercially under their proper chemical name, often not offered at all, but may be prepared and used by the interested company for "captive" use.

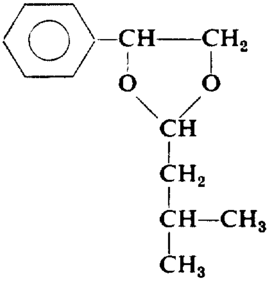
The subject acetal is not one of the more interesting ones, but it could introduce pleasant modifications of Fougères, Lavender, New Mown Hay bases, etc.

Prod.: by condensation of *n*-Valeric aldehyde with *n*-Amylalcohol. Variations are obtained by the use of *iso*-Valeric aldehyde and/or *iso*-Amylalcohol.

31-72; 37-281;

## 3055: iso-VALERALDEHYDE PHENYLETHYLENEGLYCOL ACETAL

*iso*-Amylidene-phenylglycolacetal.
2-*iso*-Butyl-4-phenyl-*meta*-dioxolan.



$C_{13}H_{18}O_2 = 206.29$

Colorless viscous liquid.

Slightly soluble in water, soluble in alcohol and oils.

Heavy, herbaceous-earthy, but overall sweet and tenacious odor. Samples of different origin have shown considerable difference in odor characteristics.

The title material is not commonly offered under its proper chemical name, but often manufactured by the interested party for captive use in perfume and flavor bases. It is, in the author's opinion, not as interesting as the Acetal made with Propylene glycol or Ethylene glycol.

Prod.: by condensation of *iso*-Valeric aldehyde with Phenylethylene glycol preferably using a catalyst (Phosphoric acid, etc.) and a low-boiling solvent for azeotropic removal of water. *iso*-Valeric aldehyde itself is very inclined to form azeotropes with various solvents, including water, and the water-carrier solvent should be selected for the purpose.

## 3056: n-VALERIC ACID

Pentanoic acid.
Propylacetic acid.
Valerianic acid.

The name "Valeric acid" is commonly used also for the *iso*-Valeric acid, see next monograph, in fact, the latter is probably the more common of the two.

$CH_3(CH_2)_3COOH$

$C_5H_{10}O_2 = 102.14$

Colorless liquid. Sp.Gr. 0.94. B.P. 186° C.

3.5% soluble in water, miscible with alcohol, Propylene glycol and oils.

Very powerful and penetrating, diffusive, acid odor, pungent when undiluted, but more unpleasant when diluted. In fact it becomes more animal- and perspiration-like in dilution. Only in extreme dilution the odor becomes again more pleasant, fruity, warm.

The taste at concentrations lower than 10 ppm is rather fruity and not really unpleasant. Higher concentrations tend to produce an odor, which makes the taste impression more unpleasant.

The title material is very rarely used in perfumes. It is occasionally used in minute traces in artificial essential oils, flower absolutes, Civet bases, etc.

It finds extensive use, although always in minute concentrations, in flavor compositions, such as imitation Butter, Cheese, Coffee, Strawberry, Rum, etc. in Butterscotch flavor, fruit complexes, etc. Concentrations in finished products are usually about 1 to 8 ppm.

The lower esters of Valeric acid, including the Methylester, are frequently used in flavors, and it must be expected that these will hydrolyze to some degree, and produce small amounts of Valeric acid. This secondary effect may or may not be desirable. In total absence of water, acid and alkali, these esters are generally very stable, provided they are acid-free in the first place. Higher esters of Valeric acid show very little tendency of becoming hydrolyzed.

Prod.:

1) by oxidation of *n*-Pentanol.
2) by fermentation process.

G.R.A.S. F.E.M.A. No.3101.

66-572; 90-69; 100-1086; B-II-299;

## 3057: iso-**VALERIC ACID**

*3*-Methylbutyric acid.
*iso*-Pentanoic acid (see NOTE).
*beta*-Methylbutyric acid.
*iso*-Butylformic acid.
*iso*-Propylacetic acid.
Delphinic acid.

NOTE: A third isomer is included in this work under the name: *alpha*-Methylbutyric acid.

$(CH_3)_2CH—CH_2—COOH$

$C_5H_{10}O_2 = 102.14$

Colorless liquid. Sp.Gr. 0.93. B.P. 176° C.

4% soluble in water, miscible with alcohol, Propylene glycol and oils.

Very diffusive, acid-acrid, in moderate dilution cheesy, unpleasant odor of poor tenacity – although the difficulty in removing minute traces from the human skin, and the power of the odor, give impression of considerable tenacity. In extreme dilution the odor becomes more agreeable, herbaceous, more dry than the odor of the *n*-Valeric acid.

The title material is very rarely used in perfumes.

It finds some use in flavor compositions, generally for the same purposes as mentioned under *n*-Valeric acid, except that the *iso*-Valeric acid is more useful in Nut and Coffee imitations due to its peculiar warm-herbaceous taste in concentrations lower than 20 ppm.

Concentrations of this acid in finished products may be about 1 to 16 ppm.

G.R.A.S. F.E.M.A. No.3102.

Prod.: (several methods) e.g. by oxidation of *iso*-Pentanol (and also from Fusel oil).

1-202; 66-572; 90-72; B-II-309;

## 3058: iso-**VALERIC ANHYDRIDE**

*iso*-Valeric acid, anhydride.

$[(CH_3)_2CH—CH_2—CO]_2O$

$C_{10}H_{18}O_3 = 186.25$

Colorless liquid. Sp.Gr. 0.93. B.P. 215° C.

Slightly soluble in water (decomposes), soluble in alcohol and oils.

The title material is briefly mentioned because it has occasionally been used in perfumery in a rather unconventional manner.

Its odor is very pungent, acrid, offensive, dry-sour, and the taste is similar to that of *iso*-Valeric acid (decomposition to acid in water).

The presence of even small amounts of this material in a perfume composition containing a large amount of alcohols (from a chemical point of view) may cause a relatively rapid esterification of a certain amount of these alcohols, selected by affinity to the anhydride.

The process could be described as an intentional ageing process, only the anhydride has been deliberately introduced, and it will eventually produce valerates of alcohols in the fragrance, with little control exercized by the perfumer. The result may not be unpredictable, but it is hardly reproducible.

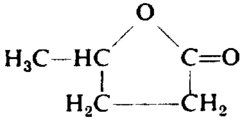
The author finds that this is "the hard way" of introducing trace amounts of valerates in a composition, and the process is not completely under control for time or for perfection.

The material is therefore mentioned mostly as a curiosity in perfumery. It is widely used for making useful esters of *iso*-Valeric acid for perfumes and flavors.

66-587; B-II-314;

## 3059: gamma-**VALEROLACTONE**

Pentyllactone.
Pentanolide-*1*:*4*.
*3*-Valerolacetone.
*3*-Methyl-*n*-*gamma*-butyrolactone.
*gamma*-Valeryllactone.



$C_5H_8O_2 = 100.12$

Colorless oily liquid. Sp.Gr. 1.05.
B.P. 207° C.

Miscible with water, alcohol, Glycerin, Propylene glycol and oils.

Warm, sweet, Hay- and Tobacco-like, herbaceous odor of moderate to poor tenacity.

Very sweet, warm-herbaceous, mildly spicy taste at concentrations lower than 100 ppm. The material has a considerable range of "pleasant concentration" and the upper limit for pleasant taste impression is very high, but the taste effect and power is not very great.

This lactone has found considerable use in perfume formulations, where its warm-herbal notes are compatible with many floral notes, e.g. Jasmin (in which Tobacco notes are often desirable).

It gives interesting effects in Fougères with Oakmoss and Coumarin, and it blends well with the herbaceous oils, particularly with Clary Sage and Todd oil No.664 (Mentha Citrata No.664). It is also interesting for novel modifications of the "Oriental fragrance" theme.

The material finds extensive use in flavor compositions, particularly in Vanilla, where it introduces support to the very natural "pungency" of the flavor, a mild sort of peppery effect, sometimes introduced with Castoreum and Zingerone. It is also used in tobacco flavorings. Concentrations in finished products vary from 5 to 50 ppm.

G.R.A.S. F.E.M.A. No.3103.

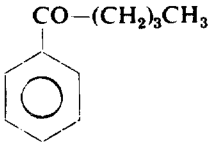
Prod.:

1) from Vinylacetic acid via Bromobutyric acid.
2) by hydrogenation of Levulic acid over Platinum in Ether.
3) by reduction of Levulic acid in presence of Raney-Nickel catalyst.
4) from Pentane-*1*:*4*-diol by dehydrogenation.

31-163; 66-795; 66-799; 106-341; 140-153; 159-419; 163-75;

## 3060: VALEROPHENONE

Phenyl butyl ketone.
Butyl phenyl ketone.
*1*-Phenyl-*1*-pentanone.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid, solidifying in the cold. B.P. 240° C. Sp.Gr. 0.99.

Insoluble in water, miscible with alcohol and oils.

Fresh-fruity, also sweet and discretely floral odor of moderate tenacity.

Sweet-fruity taste with a herbaceous note in concentrations lower than 20 ppm. The taste becomes rather unnatural-perfumey at concentrations higher than 100 ppm.

The title ketone has been suggested for use in perfume compositions, and it has some effect upon fruity-floral fragrance types, although its direct odor contribution is not very great.

The odor description "balsamic Valerian" is repeatedly quoted in literature, probably requoted without further testing, and the author of this work does not agree with that odor description. There is even a hazard of confusion with other chemicals. Unfortunately, this material has sometimes been confused with Valerolactone (see monograph) which is an entirely different chemical and has entirely different organoleptic properties.

The title ketone is occasionally used in imitation Strawberry, Peach, Cherry and other fruit flavors, but the author finds that the effect is not nearly as interesting as that of the remotely related, higher homologue. Benzyl dipropylketone (Morellone) – see that monograph.

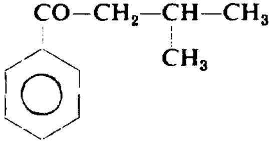
Prod.:

1) by reduction of Butyl phenyl carbinol.
2) from Benzonitrile and Butyl magnesium chloride, followed by hydration.

31-83; 36-1258; 68-532; 163-63; B-VII-327;

## 3061: iso-VALEROPHENONE

Phenyl-*iso*-butylketone.
*iso*-Butyl phenylketone.
*3*-Methyl-*1*-phenyl-*1*-butanone.



$C_{11}H_{14}O = 162.23$

Colorless oily liquid. Sp.Gr. 0.99.
B.P. 237° C.

Insoluble in water, soluble in alcohol and oils.

Fresh-fruity, sweet and moderately tenacious odor. The fruity notes are fresher, less floral than those of the *n*-Valerophenone.

The title material has been suggested for use in perfume compositions. If it were available at a cost competitive to that of the large-volume soap-fragrance chemicals, it could undoubtedly find extensive use as a sweetener and modifier in many fragrance types, floral and non-floral. It is very stable in alkali, and compatible with most of the conventionally employed soap fragrance chemicals.

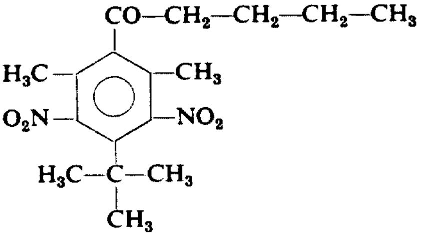
The author is not aware of any use of this material in flavors, although the *n*-Valerophenone has been suggested for that purpose.

Prod.:

1) from *iso*-Butyl phenylcarbinol by reduction.
2) from Benzonitrile plus *iso*-Butyl magnesium chloride, followed by hydration.

31-83; 68-532; B-VII-329; 86-73;

## 3062: VALERYLDINITRO-tertiary-BUTYL-meta-XYLENE



$C_{17}H_{24}N_2O_5 = 336.40$

Yellowish crystals. M.P. 151° C.

Insoluble in water, soluble in hot alcohol and most oils.

This Nitromusk was developed after the success of its lower (3 carbons lower) homologue, Musk Ketone.

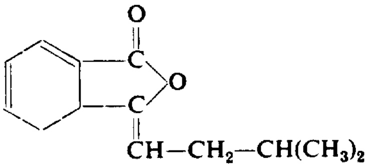
Although it has a very strong and acceptable musk odor, its production cost does not warrant any further encouragement to use this musk. It could never compete with Musk Ketone in cost, and it does not outperform that musk in use.

The title material has only academic interest today, and it has also served to prove that the change in the Nature of the acyl-radicle does not seriously influence the musk odor.

Prod.: parallel to that of Musk Ketone (see monograph) but using Valeroylchloride in place of Acetyl chloride.

5-300; 159-634;

## 3063: 3-iso-VALIDENE-3a,4-DIHYDROPHTHALIDE



$C_{13}H_{16}O_2 = 204.27$

Pale yellowish, oily liquid. B.P. 282° C.

Very slightly soluble in water. The aqueous solution (e.g. 0.1 %) has a conspicuous green fluorescence.

The odor is heavy-pungent, warm, spicy, rather unpleasant in the pure state, but becomes very attractive, agreeable at lower concentrations, clearly resembling the odor of Celery.

The taste is slightly burning at concentrations higher than 5 ppm, and it is most pleasant, Celery-like, non-bitter, at concentrations near 1 ppm. In combination-spices, however, the slight bitterness can be overcome, and the pleasant-level of the title material will be somewhat higher.

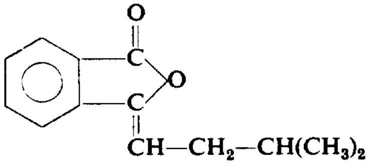
The subject lactone is one of many identified in natural products over the past decade or two. Many of these materials have been synthesized, but few are commercially available. Certain very strongly interested users may prepare their own materials, and not offer them for sale.

Prod.:

1) by isolation from Celery seed oil.
2) synthetic – from Phthalic anhydride.

90-630; 158-146;
See also: Journal of Organic Chemistry, vol. 28, 1963, page 985.
Journal of Food Science, vol. 28, 1963, page 640.

## 3064: 3-iso-VALIDENE PHTHALIDE



$C_{13}H_{14}O_2 = 202.26$

Pale yellowish oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

The solutions show a beautiful bluish-green fluorescence in dilution. Warm-herbaceous, spicy and very tenacious odor, in extreme dilution resembling Celery, but in the concentrated form rather unpleasant, pungent-

"burnt". Overall more pungent than the -dihydrophthalide (see previous monograph).

The taste at concentrations lower than 10 ppm is Celery-like, but slightly bitter, distinctly burning at higher levels. The pleasant level is near 1 ppm, and the "Minimum perceptible" lower than 0.1 ppm.

The title material has come into the limelight of the flavor laboratories since it was identified in Celery oil along with several related chemicals, many of which have been synthesized.

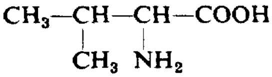
Although not a commercially available chemical, the subject lactone may be synthesized by various interested users for their own flavor composition use.

Prod.:
1) by isolation from Celery seed oil.
2) synthetically – starting from Phthalic anhydride.

90-630; 158-146;
See also: Journal of Organic Chemistry, vol. 28, 1963, page 985.
Journal of Food Science, vol. 28, 1963, page 640.

## 3065: VALINE

*L*-Valine. (*DL*-Valine included in this description).
*alpha*-Amino-*iso*-valeric acid.
*2*-Amino-*3*-methylbutanoic acid.



$$\underset{\displaystyle CH_3}{CH_3-CH}-\underset{\displaystyle NH_2}{CH}-COOH$$

$C_5H_{11}NO_2 = 117.15$

Leafy crystals. M.P. 315° C (under decomposition).

9% soluble in water, practically insoluble in alcohol and oils.

The pure material is virtually odorless, and has only a mild, warm, breadlike taste, varying from slightly unpleasant (towards stale bread) to quite agreeable.

This material is not used in perfumes.

It finds extensive use in foods as a nutrient-additive, not solely as a flavor, and not incorporated in the flavor composition if such material is used. Valine is included in this work because of its substantial interest to modern food chemistry and technology, and because the use of Valine in a food product may significantly influence its flavor, and thereby affect the work of the flavorist who will supply the flavor to the same food product.

As a nutrient, Valine is used at the rate of 1 to 2 grams per day, and may therefore constitute a large proportion of a food product.

G.R.A.S. (by the American F.D.A.).

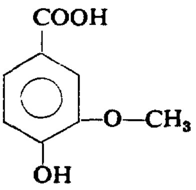
Prod.:
1) from Ammonia and Hydrocyanic acid plus *iso*-Butyric aldehyde via the Nitrile, followed by hydrolysis (Strecker synthesis).
2) Valine can also be isolated from fish proteins.

See also: Aminobutyric acid.

1-292; 66-829; 100-1087;

## 3066: VANILLIC ACID

*para*-Hydroxy-*meta*-methoxybenzoic acid.
*4*-Hydroxy-*3*-methoxybenzoic acid.



$C_8H_8O_4 = 168.15$

White or colorless, needle-like crystals. M.P. 211° C.

Sublimes when heated.

0.2% soluble in water, soluble in alcohol and oils.

Virtually odorless when pure. Slightly bitter taste in aqueous solution.

The title acid is briefly mentioned here because it represents one of the decomposition products of Vanillin when that material is exposed to oxidation. In other words, Vanillin may "lose odor" when exposed to air.

The material, as such, has probably no application in perfumes or flavors.

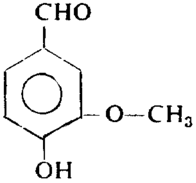
Prod.:

1) by oxidation of Vanillin.
2) by controlled fusion of Vanillin with Potassium hydroxide at 220-230° C.

68-775; 90-513; 100-1089; B-X-392; 156-351;

## 3067: VANILLIN

*4*-Hydroxy-*3*-methoxybenzaldehyde.
Methyl protocatechuic aldehyde.
Protocatechu aldehyde methylether.
"Vanillic aldehyde".
"Lioxin" (a brand of crude Vanillin, Ontario Paper Company, Ltd.).



$C_8H_8O_3$ = 152.15

White or creamy-white needle-like crystals. M.P. 83° C. (commercial grades often 81° C.). Sublimes when heated.
Sp.Gr. 1.06 (liquid). B.P. 285° C (in $CO_2$-gas).

Intensely sweet and very tenacious creamy-Vanilla-like odor. The use of the word "Vanilla" is more or less forced, and not very descriptive since – today – so many people are living without ever seing or smelling a Vanilla bean (pod). The "Vanilla" in their mind, is actually derived from a Vanillin-flavored product (Chocolate, Icecream, etc.) and it is not surprising that the Vanillin smells of Vanillin!!

A typical example of human deficiency in odor description. A common remark from laymen, smelling highly diluted Vanillin is "Chocolate", often the first reaction to the odor of Vanillin.

However, the "creamy" effect of Vanillin in trace amounts in perfumes is rather typical. Higher proportions often cause sickening sweetness and very conspicuous notes in the dryout (terminal odor).

1% soluble in water, 5% soluble in Glycerin, soluble in Propylene glycol, alcohol and oils. Vanillin is easier soluble in diluted alcohol than in concentrated alcohol. A similar situation is observed with the Glycols.

Among the more common perfume materials, Vanillin is one of the most tenacious odors known. Statisticians have often amused themselves – and some readers – with figures of how small amounts of Vanillin the human nose can detect. Most of the figures quoted, derive from an investigation of Katz and Talbert in 1931, and the author would prefer to see newer confirmation of these very questionable figures, before making any repeated quoting of such old findings. (See literature 159-146).

As a companion to the conventional "crystals" in ordinary perfume formulations, Vanillin is very widely used. It is practically always the smaller (amount) of crystalline materials, but the frequency of its use, combined with its enormous use in flavors, make it one of the largest volume, crystalline aroma-chemicals. Its intense sweetness is utilized in industrial masking odors and in high-cost luxury perfumes, and it can be used in almost any type of fragrance, from woody or herbaceous to Oriental or floral.

As a result of the volume of Vanillin produced, considerable research has been spent on perfecting the material, and it is one of the purest perfume and flavor chemicals – from a chemical point of view. While Vanillin has been improved, so has many raw materials for the functional products. And this may be part of the reason why Vanillin is no longer the considerable "hazard" in a soap perfume as it was ten or twenty years ago. The soap has been vastly improved, and so has Vanillin. It does not discolor a soap today to the degree it would have done in a soap 20 years ago.

This should not be translated so that Vanillin is not an "offender" in a soap perfume. It still is, but just not a very serious one.

Vanillin will often produce off-color with Anthranilates, Indole, Quinolines, etc. and with traces of Iron (e.g. from crude essential oils or Resinoids). However, normal use levels of the material cause very little trouble in perfumes or functional products. Certain perfume types may have exceptionally high proportions of Vanillin (5 to 8%) and such perfumes can rarely be used in white functional products (creams, handlotions, etc.), but they may be acceptable in pink or cream-colored products, where a slight discoloration from the Vanillin would not be visible.

As a masking agent for numerous types of ill-smelling, mass-produced industrial products, particularly those of synthetic rubber, plastic or fiberglass, etc., Vanillin finds very extensive use. It is often the most inexpensive material for the amount of masking effect it gives. Crude Vanillin is acceptable for such purposes.

In flavor compositions, Vanillin is used widely as a sweetener, not only in Vanilla imitation flavor, but in Butter, Chocolate, all types of fruit and tutti-frutti flavors, root-beer, "Cream-soda" etc. It is acceptable at widely different levels of concentration, and while 50 to 1000 ppm is quite normal levels in the above types of product (finished products) concentration up to 20,000 ppm (one part in fifty parts of finished goods) are also used for direct consumption (toppings, icings, etc.). Icecream and Chocolate are among the largest outlets for Vanillin in the food and candy industries, and their consumption is many times larger than that of the perfume industry.

The literature is abundant with information on the subject of Vanillin, its manufacture, uses, statistics, etc. and the interested reader is referred to such works for more complete information. It may be illustrative however, to briefly mention that Vanillin cost 8750 Francs per kilo in 1876, 875 Francs in 1886 and 155 Francs in 1897.

A French book, published more than 70 years ago on the subject of certain flavor chemicals, spends 66 pages on Vanillin and describes 39 patented methods for its manufacture.

The author of this work has preferred to mention only a few of the most important methods of production:

1) from Lignin. In principle it is the very first method commercially used. It is based upon the utilization of the glucoside Coniferin, which can be hydrolyzed to yield Coniferyl alcohol. This alcohol can be oxidized to yield Vanillin (and Acetaldehyde). Coniferin is also known as Abietin. Naturally occurring Lignin is enzymatically decomposed to give various products, one of which is Coniferyl alcohol.
2) from Guaiacol. This is the only truly synthetic method of importance. All other methods are based upon a natural starting material, closely related to Vanillin in chemical structure.

   The reaction includes Chloroform and alkali (old method) or Chloral (= Trichloro acetaldehyde), followed by oxidation of the resulting chlorinated carbinol, and hydrolysis to yield Vanillin.
3) from Eugenol. The method usually goes via *iso*-Eugenol, which is acetylated to Acet-*iso*-eugenol. Oxidation and hydrolysis yield Vanillin.
4) from Protocatechu aldehyde. Simple Methylation yields Vanillin, but the material is often accompanied by *iso*-Vanillin.
5) from Safrole. The method has great importance where Safrole-bearing essential oils are abundant and inexpensive (Japan). The process goes via *iso*-Safrole and *iso*-Eugenol to Vanillin. This process, too, may yield some *iso*-Vanillin, since *iso*-Chavibetol is formed parallel to the *iso*-Eugenol in the process.

Method No.1 is by far the most important today. A certain amount of Vanillin "ex Eugenol" is specifically requested by the flavor industry, or by flavor houses insisting upon a "very natural Vanillin". The production of Vanillin from Lignin has come to such perfection that a cream-colored product (from Lignin) can sell as "Vanillin ex Eugenol". The industry expects the latter type to be off-white or cream-colored, while Lignin-Vanillin is practically snow-white.

It is possible to smell a difference in the

Vanillins of different origin, but it is normally very difficult to taste a difference, provided the various samples are of otherwise good quality. Adherent or adsorbed odor upon the crystals will perceptibly affect the odor of Vanillin out of a fibre-drum or other large container, and the material is very sensitive to contamination with other crystalline odor chemicals. An admixture of 0.05% Coumarin to Vanillin will introduce an entirely different odor, conspicuous to the layman. Yet, Vanillin is considered a more powerful odorant than Coumarin.

The taste effect is generally sweet, but it depends greatly upon the base. Vanillin for flavor purposes is often evaluated in ice cold milk, sweetened with about 12% sugar. Concentrations of 50 ppm in this medium are clearly perceptible and will not fatigue the evaluator.

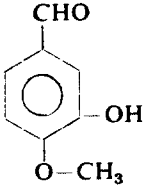
1-514; 5-126; 31-53; 31-61; 68-746; 72-111; 85-119; 90-503; 95-142; 96-128; 100-1089; 103-252; 104-645; 106-342; 140-128; 140-162; 156-344; 159-466; 163-75; 163-243; B-VIII-247;

G.R.A.S. F.E.M.A. No.3107.

See also: Coniferyl alcohol.

## 3068: iso-**VANILLIN**

*3*-Hydroxy-*4*-methoxy benzaldehyde.
*para*-Monomethyl protocatechualdehyde.



$C_8H_8O_3 = 152.15$

Colorless crystals. M.P. 117° C.
Sp.Gr. 1.19 (liquid). B.P. 282° C.

Slightly soluble in cold water, soluble in hot water, alcohol and oils. Sublimes when heated.

Practically odorless when cold; mild, floral-herbaceous or Hay-like at room temperature, and very sweet, balsamic-Vanilla-like when heated above 60° C.

Although there may well be differences of personal opinion as to the exact odors at various temperatures, it seems beyond doubt that this material displays quite a range of slightly different odors as it is heated from 0° to less than 100° C.

The change in odor from 0 to 20° C. is not a rare occurrence, and most perfumers have undoubtedly made that observation, but the continuation in change to the distinctly Vanilla-like is rather unusual and specific for this material.

The material as such is rarely used in perfumes or flavors, since its aromatic value is too inconspicuous, but it has some importance since it occurs along with Vanillin in one of the many processes used for the manufacture of that important material.

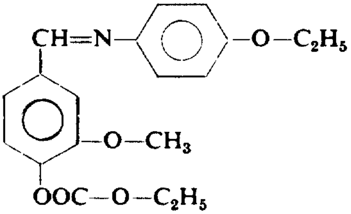
Prod.:

1) by Methylation of Protocatechualdehyde. Some Vanillin is also formed.
2) by oxidation of Hesperitic acid.

1-513; 5-128; 31-39; 68-747; 72-147; 90-514; 96-138; 140-278; 163-243;

## 3069: VANILLIN-ETHYLCARBONATE-para-PHENETIDINE

Vanillin-*para*-phenetidine ethylcarboxylate. "Eupyrin".



$C_{19}H_{21}NO_5 = 343.39$

Yellowish needle-like crystals. M.P. 88° C.

Very slightly soluble in water, moderately soluble in alcohol, soluble in hot alcohol and oils.

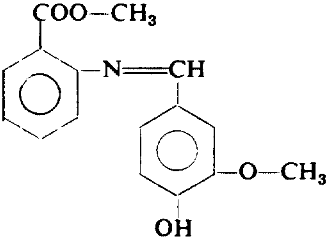
The title material is briefly mentioned because it behaves in a rather peculiar manner. Although it has an unquestionable odor of Vanillin-type, rather soft, but quite pleasant and not exactly weak, its aqueous solution or the dry material itself has hardly any taste at all.

This peculiarity has not been explained in literature, but it could well be that the material (molecule), part of which is an aromatic aminoether, has mildly anaesthetic effect upon the human mucous membranes. Many members of this chemical series have anaesthetic effect.

The material was developed many decades ago for pharmaceutical purposes, but was also introduced to the perfume and flavor industry at that time. It has no longer importance to perfumes or flavors, but it is still used in pharmacy.

96-137; 100-411;

## 3070: VANILLIN-METHYLANTHRANILATE



$C_{16}H_{15}NO_4 = 285.30$

Viscous, dark-yellowish liquid, occasionally with an orange-reddish tint, or an olive-green color.

Insoluble in water, soluble in alcohol and oils.

Intensely sweet, balsamic-floral odor of very good tenacity. The odor varies considerably from one sample (supplier) to another, a fact which is often observed in "Schiff's bases". Generally, a mild surplus of the aldehyde component is preferable, except in cases of very pungent aldehydes such as Cuminaldehyde, Cinnamic aldehyde, Methylcinnamic aldehyde, etc.

The title material has very little use in perfumes, and is simply missing from most perfume laboratories. It may be considered as a curiosity, more than a practical perfume material, but it is briefly mentioned in this work because it may often "occur" in a perfume, since the use of Vanillin and Methylanthranilate in the same composition is not a very rare or unusual case. The addition of Vanillin directly into Methylanthranilate may often cause a strong coloring, brown or orange, of the mixture, and it is recommended not to add these materials in sequence, one next to the other.

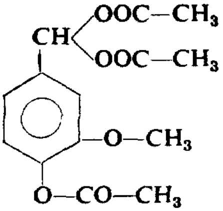
Among scores of suggested "Schiff's bases", only very few have become standard perfume items, and the title material is not one of them. But it is classified as "interesting", by some perfumers.

Prod.: by condensation of Vanillin with Methylanthranilate in molecular proportions, preferably in a suitable diluent to prevent violent darkening, and to render the final product more pourable, handy for use.

33-1029; 90-799;

## 3071: VANILLIN TRIACETATE

Acetylvanillin diacetate.



$C_{14}H_{16}O_7 = 296.28$

White needle-like crystals. M.P. 89° C.

Poorly soluble in water, soluble in alcohol and oils.

Practically odorless and tasteless.

This material is briefly mentioned in this work in order to complete the description of acetylated Vanillins, the nomenclature of which is rather confused in the perfumery literature.

It has often been claimed that the Hydroxyl group is necessary in the Vanillin molecule to supply the Vanilla-like odor type and the power. It could be expected that a completely "neutralized" molecule like the above is of little or no odor.

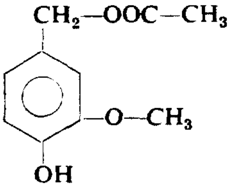
Prod.: from Vanillin in alkaline solution with surplus of Acetic anhydride and Sodium acetate. Also by dry reaction upon an alkaline salt of Vanillin.

72-152; 90-513; 156-351;

See monograph on Acetylvanillin, listing five related materials.

## 3072: VANILLYL ACETATE

The acetate of Vanillyl alcohol.



$C_{10}H_{12}O_4 = 196.21$

Colorless or white crystals.

Very slightly soluble in water, soluble in alcohol and oils.

Mild, sweet-balsamic, delicately floral odor of good tenacity. The odor has only little in common with the Vanilla-odor, and it does not have the deep warmth of Vanillin.

This material has occasionally been used in perfume compositions as a modifier for Vanillin or for Anisylesters in perfumes of the "powdery" fragrance type, sweet and delicate florals, etc.

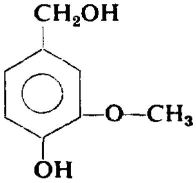
It is relatively expensive and its effect is not one of great power. Since the perfumer has a large number of materials with similar effect at lower cost, the title material will most likely remain a curiosity and not become a useful perfume material.

Prod.: from Vanillin by electrolytic reduction, followed by Acetylation of the Vanillyl alcohol.

156-350;

## 3073: VANILLYL ALCOHOL

*4*-Hydroxy-*3*-methoxybenzylalcohol.



$C_8H_{10}O_3 = 154.17$

White or colorless crystals. M.P. 115° C. Decomposes before melting.

Almost insoluble in cold water, soluble in hot water, alcohol and oils.

Very mild, sweet, balsamic-Vanilla-like odor of moderate tenacity. Oxidation produces Vanillin, and the odor intensity increases accordingly if the material is exposed to air.

The title alcohol is briefly mentioned in this work, partly to complete the description of materials closely related to Vanillin, partly because it has had some use in perfumes and flavors, many years ago, when the price difference between the alcohol and Vanillin was not very significant.

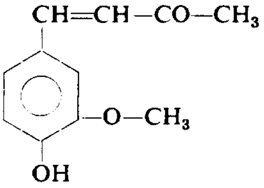
But since the material is primarily made from Vanillin, and since it has much less odor- and flavor value, it has become practically obsolete today.

Prod.: from Vanillin by hydrogenation in presence of Platinum black.

68-737; 90-513; 163-75; B-VI-1113;

## 3074: VANILLYLIDENE ACETONE

Vanillal acetone-(*1*,*3*,*4*).
Ferulic methyl ketone.
*4*-(*4'*-Hydroxy-*3*-methoxyphenyl)-*3*-buten-*2*-one.



$C_{11}H_{12}O_3$ = 192.22

Yellowish, needlelike crystals. M.P. 130° C.

Slightly soluble in water, soluble in alcohol and oils.

Very sweet, warm and tenacious odor of balsamic-creamy Vanillatype, although more spicy, less delicate than Vanillin.

The title material was suggested for use in perfumes and flavors many years ago, but has apparently failed to obtain a space on the perfumer's shelf. It is relatively unstable, prone to oxidation and polymerization, but would not deteriorate in a perfume composition at normal use level of dilution.

The material is still produced as an intermediate in the manufacture of Zingerone (see monograph), and it can also be hydrogenated under different circumstances to Homoeugenol.

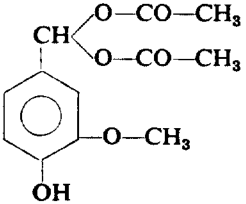
It is related to Coniferaldehyde (one of the chief flavor ingredients in Maple syrup) in that the title material is prepared by condensation of Vanillin and Acetone under alkaline conditions, while Coniferaldehyde is prepared from Vanillin and Acetaldehyde under similar conditions.

See also Conifer aldehyde.

26-716; 68-989; 163-382; B-VIII-291;

## 3075: VANILLYLIDENE DIACETATE

"Vanillin diacetate".



$C_{12}H_{14}O_6$ = 254.44

White or colorless crystals.

Very slightly soluble in water, soluble in alcohol and oils.

Very faint, sweet-floral, refreshingly delicate odor of good tenacity.

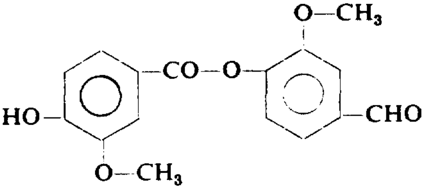
The odor of this material is not sufficiently powerful or interesting that it can be included as a perfume chemical.

The title material is mentioned briefly to complete the description of the acetylated Vanillins.

See also the monograph on Acetyl vanillin for summary of acetylated Vanillins.

## 3076: VANILLYL VANILLATE

Vanillic acid, vanillylester.



$C_{16}H_{14}O_6 = 302.29$

Colorless or white crystals.

Very slightly soluble in water, fairly soluble in hot water, soluble in alcohol and oils.

Warm and sweet, Vanilla-like odor, stronger than Vanillin, but weaker than "Ethyl vanillin".

Among numerous derivatives prepared in the Vanillin family, this is one member of sufficiently interesting odor that it should be mentioned and tested. It has been known for many decades, but since the synthesis of this material is more complicated than that of Vanillin and "Ethyl vanillin", there has been considerable reluctance in promoting this ester.

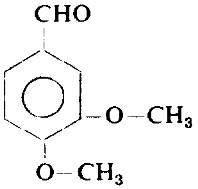
It carries the same type of sensitivity to alkali and iron metal as Vanillin, and therefore has no apparent advantage.

It is quite possible that the title ester is used as a modifier in Vanillin-compositions for imitation Vanilla – outside of the USA.

28-549;

## 3077: VERATRALDEHYDE

*para*-Veratric aldehyde.
*3,4*-Dimethoxybenzaldehyde.
Protocatechualdehyde dimethylether.
Methyl vanillin.
"Methyl protechin".
Vanillin methylether.
*3,4*-Dimethoxy benzenecarbonal.



$C_9H_{10}O_3 = 166.18$

White crystals, or cream-colored, fused mass. M.P. 44° C. B.P. 281° C. The liquefied material will often remain supercooled at room temperature for a considerable length of time before it crystallizes. Sp.Gr. 1.15 (liquid).

Almost insoluble in cold water, soluble in hot water, alcohol and oils. Under exposure to air and daylight, the material may oxidize to an odorless acid (Veratric acid).

Very sweet, woody-Vanilla-like or Heliotrope-like odor of excellent tenacity. Some observers find a haylike or Coumarin-like note in this material.

Warm and sweet-herbaceous Vanilla-like taste in concentrations below 40 ppm. The flavor effect is similar to that of Heliotropine, but not nearly as "perfumey". Veratraldehyde is not frequently used in perfumes. The mediocre grade often offered commercially has a poor appearance and may have contributed to an initial aversion against this aldehyde. It does have some disadvantage in discoloring under alkaline conditions, but not more so than Vanillin. A pure grade of Veratraldehyde is an excellent perfume material with more warmth and depth than Vanillin, and excellent effect in "Oriental" type fragrances, woody-musky bases, etc. It is also an interesting variation of – or companion to – Anisaldehyde.

The material finds some use in flavor compositions, mainly in imitation Vanilla, Nut and Butterscotch, but also in various fruit complexes. The concentration used is normally about 10 to 30 ppm in the finished product.

Prod.: by Methylation of Vanillin with Dimethylsulfate in mild aqueous alkali.

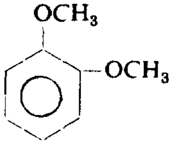
G.R.A.S. F.E.M.A. No.3109.

1-890; 13-84; 36-1027; 34-787; 68-747; 90-528; 100-1091; 163-243; 163-382; B-VIII-255; 140-279;

See also: Homo veratraldehyde (*3*-Methoxy-*4*-ethoxybenzaldehyde, sometimes called Methyl-*iso*-ethylvanillin).

## 3078: VERATROL

Catechol dimethylether.
Pyrocatechin dimethylether.
*ortho*-Dimethoxybenzene.



$C_8H_{10}O_2 = 138.17$

Colorless viscous liquid, fused opaque mass, or crystals. M.P. 23° C. Sp.Gr. 1.09 (liquid). B.P. 207° C.

Very slightly soluble in water, soluble in alcohol and oils.

Sweet-creamy, rather pungent odor which upon dilution becomes very Vanilla-like.

Earthy-sweet, Nut-like, but very sweet and also Vanilla-like taste in concentrations below 20 ppm.

The title chemical is rarely offered from the usual manufacturers of perfume and flavor chemicals, but it is often prepared by the interested party for use and not re-sale. It could be used as a modifier in Oakmoss compositions and artificial Oakmoss bases, and it blends very pleasantly with Coumarin, Vetiver, Amylsalicylate, etc. in fixative bases for Colognes, etc.

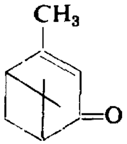
The ether has been suggested for use in flavor compositions, e.g. Nut, Walnut, Vanilla, etc. but it is not included in the American G.R.A.S. list and probably not used in the USA for food flavors.

Prod.: by Methylation of Catechol or Guaiacol with Dimethylsulfate in weak aqueous alkaline solution.

1-439; 31-146; 68-467; 100-1092; 163-382; B-VI-771;
For other ethers of Catechol – see under: Catechol – – –.

## 3079: VERBENONE

*2*,*6*,*6*-Trimethyl-(*1*,*3*,*3*)-bicyclohept-*2*-en-*4*-one.
*dextro*- and *laevo*-Verbenone are known.



$C_{10}H_{14}O = 150.22$

Viscous, pale straw-colored liquid, solidifying in the cold. M.P. 6° C. Polymerizes under exposure to air, becomes darker yellow, more viscous, and loses odor. B.P. 228° C. Sp.Gr. 0.97.

Practically insoluble in water, soluble in alcohol and oils.

The odor of this material varies considerably according to origin (supplier, method of production, age of material, etc.).

It is normal to find a soft, warm-resinous, slightly spicy odor of moderate tenacity, while minty-camphoraceous notes should not be dominating. The word "Celery" has often been used in the description of the odor of this material, but the author finds that it would generally be confusing, since the observer would deliberately "look for" such celery note, even if he does not find it voluntarily. But the overall impression is that of a pleasant "outdoorish" odor of resins and fresh-spicy herbs.

This material has, for some odd reason, escaped most of the perfume laboratories all over the world. The increasing number of requests for "incense" type odors, including Men's fragrances, have further promoted the search for the very few chemicals with such useful odor type. As a modifier in mildly spicy compositions, as a novel note in herbaceous-citrusy fragrances, Colognes, etc., the title ketone has unquestionable possibilities.

The simultaneous demand for "Verbena" notes has revived the interest in any material bearing the name "Verbena"- but the title material offers little, if any, help in that problem. Apart from being a useful modifier, it does not contribute any characteristic Verbena notes.

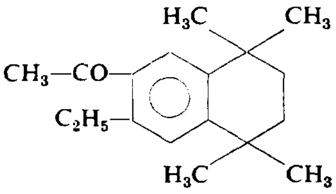
Prod.:

1) from *alpha*-Pinene by autoxidation via Verbenol to Verbenone.
2) from *alpha*-Pinene via *cis*-plus-*trans*-Pinen-*3*-ol-*2*, followed by oxidation to the title material.
3) The title material occurs in oxidized Turpentine oil.

31-89; 89-344; 95-165; 96-163; 100-1092; 163-243; 163-382; 163-76;
See also: *1,1,7*-Trimethylbicyclo-(*1,1,3*)-hepten-*1*-one.

## 3080: VERSALIDE

The title name is a trade name (Givaudan Corp.).
"Musk 36-A" is identical (trade name of U.O.P. Chemical Co.).
*1,1,4,4*-Tetramethyl-*6*-ethyl-*7*-acetyl-*1,2,3,4*-tetrahydronaphthalene.
*7*-Acetyl-*1,1,4,4*-tetramethyl-*7*-ethyl-*1,2,3,4*-tetralin.



$C_{18}H_{28}O = 258.41$

White or ivory-colored crystals, flakes or fused mass. M.P. near 43° C.

Practically insoluble in water, 8% soluble in alcohol, 10% soluble in vegetable oil, 62% in Diethyl phthalate, miscible with most perfume oils and materials.

Sweet, distinctly musky, and soft-creamy odor of good tenacity.

This Tetralin-musk is one of the most successful "non-Nitro" musks from an economical point of view. Within a ten-year period of existence on the perfumery market, it has climbed to a position among the "large-volume" selling musks. It is widely used as a musky fixative in modern soap perfumes and it has contributed to the success of several well known soaps. Yet, the research on this type and related musks continues, and improvements are still possible. The title musk is also, to a certain degree, in competition with "Galaxolide" (see monograph *1,3,4,6,7,8*-Hexahydro-*4,6,6,7,8,8*-hexamethyl-cyclopenta-*gamma*-*2*-benzopyran), of which a 50% solution is priced very near the cost of Versalide.

The title material blends excellently with sweet-woody themes, including Sandalwood and Vetiver, also Patchouli and Opopanax for "Oriental" types, and with Citrus compositions for Colognes, Men's fragrances, etc. It is less suitable for the very delicate floral types, but its greatest asset is its effect in soap and the extended retention of fragrance on the skin from a soap perfume, using this material.

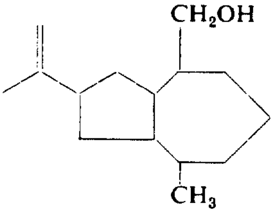
Prod.: from Ethylbenzene plus *2,5*-Dichloro-*2,5*-dimethylhexane. (Carpenter, U.S. pat. 2,897,237, 28th July 1959).

106-344; 156-281; 163-243; 163-383;
See also monographs:
Dimethyl di-*iso*-propyl indanol. (1005)
Acetyl hexamethyl tetrahydronaphthalene. (41)
Musks, summary.

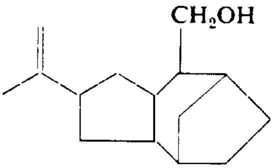
# 3081: VETIVEROL

Vetivenol.
Vetivol.
Lignolia.
- and many trade names.

The commercial product is a mixture of alcohols, isolated from Vetiver oil of different origin. Two primary alcohols constitute by far the main portion of the total alcohols isolable. Minor amounts of certain tertiary alcohols are known, but incompletely investigated. This monograph describes the average commercial product, and the formula structures below refer to the two main components in this product:



Bicyclo-vetiverol.
$C_{15}H_{26}O = 222.37$



Tricyclo-vetiverol.
$C_{15}H_{24}O = 220.36$

Sp.Gr. 1.00. B.P. 264° C.

Pale straw-colored, pale amber-colored, sometimes pale olive-green, viscous liquid. The green color comes from minute traces of Azulenes, mixed with a faint, yellow color of the product.

Practically insoluble in water, soluble in alcohol and oils. Poorly soluble in Glycols.

The odor of this product varies considerably according to origin, quality, age, etc. A warm, sweet, mildly earthy-balsamic and extremely tenacious odor is common and generally desirable. Sharp, green or pronounced "root-like" notes are generally undesirable. This material is one of the most tenacious fragrance materials known, and it is used primarily for that virtue.

Vetiverol is a relatively expensive material, and its use, often in the amount of 5 to 10% of the composition, is restricted to better perfumes (better priced perfumes). It blends particularly well with Sandalwood odors, Ionones, Styrax and various materials for "Oriental" and woody bases or perfumes. In "modern" perfumes, it finds extensive use as a fixative under mossy and certain floral bases, but it is most attractive in the non-floral types, Chypres, etc. A high grade Vetiverol will not introduce Vetiver oil notes, but only lend soft, sweet, velvety fixation.

Minor amounts of the material are used in flavors, where imitation Asparagus and Cucumber may benefit from the peculiar taste of this item. The author would however, by far recommend the lower boiling fractions of Vetiver oil for this purpose. They have an interesting green-vegetable, earthy and fresh taste, although slightly bitter, but useful for the named imitations.

Prod.:

1) by isolation from Vetiver oil, by fractionated vacuumdistillation.
2) by isolation from saponified Vetiver oil, by fractionated vacuumdistillation.
3) by treatment of Vetiver oil with Acetic anhydride, thereby acetylating the primary alcohols, and dehydrating the tertiary alcohols to hydrocarbons. Fractionated distillation isolates Vetiver acetate from primary alcohols exclusively, and subsequent saponification yields Vetiverol consisting almost exclusively of the two above named alcohols. It has been suggested, but not confirmed with certainty, that the tertiary alcohols will contribute undesirable dry-camphoraceous notes to the odor of Vetiverol.

Method No.3) yields by far the best perfumery grade Vetiverol, but it is much more expensive that the "ordinary" grades. The yield is rarely higher than 60% calculated upon the Vetiver oil, and Reunion oil (also called Bourbon oil) is still considered the superior starting material. Oils from Belgian Congo (not available since 1966), from

Angola, East India and Java have compositions entirely different from that of Reunion oil, while Haiti Vetiver oil is often considered the second best starting material for making Vetiverol. East Indian Vetiver oil is scarce outside of India, but it can give excellent Vetiverol.

The aldehydes, corresponding to the above mentioned alcohols, have been prepared experimentally, and they have been described as having Olibanum-type odor. They are not commercially available.

88-291; 103-237; 104-652; 106-348; 155-132; 163-76; 163-244;

## 3082: VETIVERYL ACETATE

Vetivenol acetate.
Vetiver acetate.
"Vetacetia" (I. F. & F.).
"Vetacetyl" (Givaudan).
"Acetivenol" (Roure-Dupont).
Vetynal.
Vetiriax.
– and many other trade names.
The trade names represent materials consisting mainly or wholly of the acetylated alcohols in Vetiver oil.

Structure and empirical formula: see Vetiverol.

Almost colorless or pale straw-colored, sometimes pale olive-green slightly viscous liquid. Sp.Gr. 1.00. B.P. 285° C.

Practically insoluble in water, soluble in alcohol and oils. Poorly soluble in Glycols.

Sweet-and-dry, fresh-woody and exceptionally tenacious odor. Poorer grades display conspicuous notes of Vetiver oil (green, earthy, rooty notes, etc.). The beauty of the odor is only fully appreciated when the material is incorporated in a suitable perfume. The peculiar dry-sweet note does not appear with a woody tone, but it gives fresh lift, yet outstanding tenacity and warmth to a fragrance. Although this ester can be used in almost any type of perfume, it has its most attractive effect in Chypres, modern aldehydic perfumes, compositions with Ionones, Opopanax, Olibanum, Orris, etc. and it is nearly perfect for powder perfumes.

Many world-wide known, very successful fashion perfumes owe part of their success to this item, although the idea of using a very large proportion of this ester in a luxury perfume is older than most of the perfumers working in today's laboratories. Which only confirms the success of the material – virtually unsurpassed through many decades.

Out of many esters prepared from "Vetiverol", this is the most important, and usually the only Vetiverylester on the perfumer's shelf. Other esters (see following monographs) have been prepared, and some are used but not sold, by creative perfume houses, for special fragrance purposes.

Prod.:

1) by Acetylation of Vetiver oil with Acetic anhydride, followed by fractionated distillation.
2) careful Acetylation of the Vetiverol, prepared by method 3) in monograph: Vetiverol, may lead to exceptionally high grade Vetiveryl acetate.
3) crude products are sometimes made by Acetylation of Vetiver oil without subsequent fractionation, but perhaps only "topping" of 5 to 10% light fractions. The product is dark and of very inferior odor.

36-484; 33-504; 103-100; 103-121; 106-346; 155-132; 163-76; 163-244;

## 2083: VETIVERYL BUTYRATE

Vetivenol butyrate.
This monograph includes the description of Vetiveryl-*iso*-butyrate. The trade rarely discriminates between the two, and uses the name "butyrate" for both, when the material is available at all.

Structure and empirical formula: see Vetiverol.

Pale straw-colored or yellowish or pale olive-green, slightly viscous liquid.

Practically insoluble in water, soluble in alcohol and oils.

B.P. 300° C. Sp.Gr. 1.00.

Fresh, yet sweet-floral, delicately fruity-oily or mildly waxy odor of outstanding tenacity. The woody notes are hardly perceptible, while the floral notes are more predominant, the fruity less so than in the Acetate.

The material is overall not very interesting, and for the very high cost of production, it does not encourage to frequent use in perfumery. It is occasionally prepared by an interested party for use in private formulations, generally not for sale.

Prod.: from purified Vetiverol and Butyric anhydride (or *iso*-Butyric anhydride).

36-484; 155-132; 163-76;

## 3084: VETIVERYL CAPRYLATE

Vetiveryl octoate.
Vetiveryl octanoate.
Vetivenol octylate.

Structure and empirical formula: see Vetiverol.

Straw-colored or very pale yellowish-greenish, slightly viscous liquid. Sp.Gr. 0.99.
B.P. over 300° C.

Practically insoluble in water, soluble in alcohol and oils.

Delicately sweet-floral, semi-dry odor with peculiar musky-animal note and outstanding tenacity.

The title ester is extremely rare, and not offered commercially. It is only occasionally prepared by an interested party for use in special fragrance creations.

The title material has very little importance in perfumery. Vetiveryl esters, in general, display the overall virtues of Vetiverol, namely outstanding tenacity with soft and discrete overall odor. The esters do offer small variations in the odor type, but the Acetate is normally the only ester found in an average perfume laboratory.

Prod.: from purified Vetiverol (see monograph, method No.3) and Caprylic acid.

163-383;

## 3085: VETIVERYL FORMATE

Vetivenol formate.

Formula and structure – see: Vetiverol.

Pale straw-colored, slightly viscous liquid. Sp.Gr. 0.99. B.P. 280° C.

Practically insoluble in water, soluble in alcohol and oils.

Delicate, dry-sweet, powdery odor of excellent tenacity. Poorly stored material often show sharp or pungent (formic) notes.

The title material is not very stable, and unless it has found steady use in a specialty composition, it will rarely be found in any perfume laboratory or stockroom. It is of very little importance to the working perfumer.

Prod.: by cold formylation of purified Vetiverol. Commercial samples have shown ester contents as low as 65%.

36-484; 155-132; 163-76;

## 3086: VETIVERYL PHENYLACETATE

Vetivenol phenylacetate.
Vetiveryl-*alpha*-toluate.

Structure and empirical formula: see Vetiverol.

Pale straw-colored or pale amber-colored, viscous liquid. Sp.Gr. 1.03. B.P. 310° C.

Insoluble in water, soluble in alcohol and oils.

Musty-sweet, mildly fruity and discretely woody-rosy odor of outstanding tenacity. Considerable variations are observed in materials of different origin.

The title ester, although very rare, is perhaps the second-most used Vetiveryl ester, after the Acetate. It finds some use as a base or "undertone" in Chypres, Oriental fragrances with Opopanax and Myrrh, Olibanum, etc. and it forms an interesting companion to Sandalwood and Patchouli, Geranium, Ionones, etc.

The ester is, however, only rarely found on the perfumer's shelf, and not used commonly in perfumery.

Prod.: from purified Vetiverol and Phenylacetyl chloride.

34-248; 36-484; 103-142; 163-76;

## 3087: VETIVERYL PROPIONATE

Vetivenol propionate.

Structure and empirical formula: see Vetiverol.

Pale straw-colored to pale yellowish, slightly viscous liquid. Sp.Gr. 0.99. B.P. 290° C.

Practically insoluble in water, soluble in alcohol and oils.

Very tenacious powdery-fruity, mildly woody odor. Not nearly as interesting as the Acetate, at least not judging from the (much fewer) samples available of the Propionate.

The title material is briefly mentioned for the sake of completion in the series of Vetiveryl esters, but the author believes that the Propionate has very little use in perfumery. It is almost never offered commercially.

Prod.: from purified Vetiverol and Propionic anhydride.

36-484; 155-132;

## 3088: VETIVERYL VALERATE

Vetivenol valerianate.

This monograph includes the description of Vetiveryl-*iso*-valerate, since the trade does not discriminate between the two esters of the alcohol in question.

Structure and empirical formula: see Vetiverol.

Pale straw-colored or pale amber-colored, slightly viscous liquid. Sp.Gr. 1.01.
B.P. 310° C.

Practically insoluble in water, soluble in alcohol and oils.

Delicately herbaceous-fruity, musty-woody, dry-and-sweet, very tenacious odor. Variations in this odor are observed when studying samples of different origin. It is quite possible that the *iso*-Valerate has a more fruity odor and the *n*-Valerate a more musty-animal, or almost musky odor, but differences occur also in the choice of Vetiverol type for the esterification, and the trade has not offered enough reliable samples that a true and unambiguous odor picture can be formed.

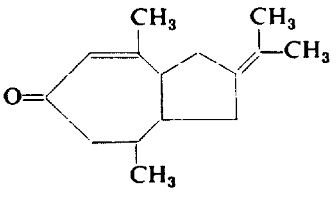
The title ester is very rare, but has found a little use in perfumery, mainly as a companion to Oakmoss- and "tabac"-notes in perfumes, including powder perfumes, where the title material performs very well.

Prod.: from purified Vetiverol with *n*-Valeric acid or *iso*-Valeric acid.

36-484; 155-132; 163-76;

## 3089: VETIVONE

Also called Vetiverone.
*alpha*-Vetivone and *beta*-Vetivone are known. Other isomers possibly exist.
*4,8*-Dimethyl-*2*-*iso*-propylidene-*6*-oxo-*cis*-$\Delta_4$-octahydroazulene.



$C_{15}H_{22}O = 218.34$

Pale yellowish or off-white crystals.
Sp.Gr. 1.00 (liquid).
M.P. 52° C. (*alpha*-Vetivone)
M.P. 45° C. (*beta*-Vetivone).

The title material represents the "ketone-fraction" of Vetiver oil, while the individual isomers are not commercial items. They have been isolated and investigated. Samples of the two named isomers are well-known and are of potential interest to the perfume industry.

*alpha*-Vetivone has a powerful, warm, pleasant, Orris-Vetiver-Ambre-like odor of outstanding tenacity. It is generally considered the most desirable odor of the two. Unfortunately, it appears to be the minor component of the total ketones in Vetiver oil.

*beta*-Vetivone has a more balsamic-floral, sweet, but very mild or relatively weak odor, although also of excellent tenacity. It is the major ketonic component of Vetiver oil.

A synthesis starting from Dimethyl-*iso*-propyl hydro-indanone may lead to the Tetrahydro-derivative of the title material, but a complete synthesis of the Vetivenones is not yet economically attractive.

By saponification of Vetiver oil, a small yield of mixed ketones can be isolated, but experiments so far have been discouraging by the fact that analysis may show a ketone content of 10 to 25% in certain Vetiver oils, while the isolable amount may be as little as 1 to 5%. The problem continues to be interesting in view of the general agreement that the ketones carry much, if not the major portion of the total odor picture of Vetiver oil.

89-433; 100-1093; 104-652;

## 3090: VINYL ACETATE

$CH_2{=}CH{-}OOC{-}CH_3$

$C_4H_6O_2 = 86.09$

Colorless mobile liquid. Sp.Gr. 0.93.
B.P. 73° C.
Polymerizes under exposure to daylight, may solidify to an odorless, brittle, almost colorless mass.

2% soluble in water, miscible with alcohol and oils.

Fruity-ethereal, rather sharp, but sweet odor of considerable diffusive power and very poor tenacity.

The title material is briefly mentioned here because it is permitted for use in food products in the shape of a modifier for food starches. Various volatile acetates are used for that purpose.

The ester, as such, has little or no application in perfumes, and probably no mission in flavor compositions.

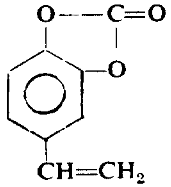
Vinyl acetate is an important chemical intermediate in the manufacture of certain Acetals, including a few perfume and flavor chemicals.

Prod.: from Acetylene plus Acetic acid over a catalyst.

66-315; 89-308; 100-1094; B-II-63 (zweiter Ergänzungsband).

## 3091: VINYL CATECHOLCARBONATE

*4*-Vinylcatechol carbonate.



$C_9H_6O_3 = 162.15$

Colorless or white crystals, becoming gray or pale amber-colored upon exposure to air. M.P. 66° C.

Insoluble in water, soluble in alcohol and oils.

Pungent, warm-spicy, but also moderately medicinal-woody odor of considerable tenacity.

The title material has been suggested for use in perfume compositions as a "leather" or "moss"-component in woody or woody-medicinal fragrance types. It could be used for the type of fragrance which is rather popular in medicinal face-cleaning creams, medicinal lotions, etc., and it has interesting effects with Oakmoss and Clove oil in spicy-mossy fixative bases for Men's fragrances etc.

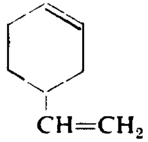
The material is rarely offered from the regular suppliers of fragrance chemicals, but occasionally from pharmaceutical-chemical manufacturers.

Prod.: by dry distillation of *3,4*-Dihydroxybenzylidene malonic acid carbonate.

68-972;

## 3092: 4-VINYL CYCLOHEXENE

*4*-Vinyl-*1*-cyclohexene.
Tetrahydro styrene.



$C_8H_{12} = 108.18$

Colorless liquid. Sp.Gr. 0.83. B.P. 126° C.

Almost insoluble in water, soluble in alcohol and oils.

Sweet-ethereal odor of poor tenacity.

The title material has been suggested for use in perfume compositions where it may introduce an acceptable form of "lift" to heavy fragrance types, balsamic or Oriental, woody, herbaceous, etc.

The hydrocarbon is actually a chemical intermediate, but has found a little use as such in industrial fragrances, low-cost masking compositions, etc.

Prod.:

1) by dehydration of *4*-Vinyl cyclohexenol with Potassium bisulfate.
2) The title material is a dimer of *1*:*3*-Butadiene.

67-142; 67-401;

## 3093: VINYL ETHYL ETHER

Ethyl vinyl ether.
(Do not confuse with Vinyl ether = Divinylether).

$CH_2{=}CH{-}O{-}CH_2{-}CH_3$

$C_4H_8O = 72.11$

Colorless mobile liquid. Sp.Gr. 0.76.
B.P. 36° C.

Very slightly soluble in water, soluble in alcohol and oils.

Very diffusive, nauseating-ethereal, but sweet odor of poor tenacity. The odor carries some similarity to that of Ethyl ether (Ether).

Aqueous solutions have a sweet taste, but not as sweet as Chloroform.

This ether is a relatively reactive chemical, and its occasional use in perfumery may just take that fact into consideration. Condensation of the title material with unsaturated alifatic aldehydes may produce very interesting and powerful perfume chemicals. In fact, the condensation product with Croton aldehyde is the first step in one of the commercial syntheses of Rose oxide.

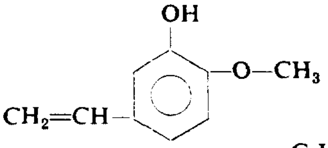
Used in very discrete amounts, the ether gives powerful lift to sweet topnotes, be it Citrus or Rose, Jasmin or "green" notes. But its affinity for unsaturated aldehydes should be kept in mind when this material is used.

Prod.: by bubbling Acetylene through Ethylalcohol in presence of Sodium ethoxide.

66-324; 90-713; B-I-433;

## 3094: 5-VINYLGUAIACOL

*4*-Vinylcatechol-*1*-methylether.
Hesperitol.
*3*-Hydroxy-*4*-methoxystyrene.



$C_9H_{10}O_2 = 150.18$

White or colorless crystals, becoming yellowish or brownish upon exposure to air.
M.P. 57° C.

Slightly soluble in water, soluble in alcohol and oils.

Balsamic-woody odor of deep sweetness, but much less spicy than *4*-Vinylguaiacol. Moderate tenacity.

The title material is very rarely offered commercially, but it has been suggested for use in perfume compositions, mainly in artificial Oakmoss bases, "leather"-notes, herbaceous-spicy fragrance types, etc.

At the present cost and poor availability, the material has almost no chance of becoming a popular fragrance chemical. And its odor type is not sufficiently interesting to encourage a search for less expensive or increased volume production.

Prod.: by dry distillation of Calcium-*iso*-ferulate (= Calcium hesperitinate), which can be obtained from *iso*-Vanillin.

68-972;
See also monograph:
*2*-Methoxy-*4*-vinyl phenol (= *4*-Vinylguaiacol) (1891).

## 3095: VINYL SULFIDE

Divinyl sulfide.

$(CH{=}CH_2)_2S$

$C_4H_6S = 86.16$

Colorless mobile liquid. B.P. 101° C.

Slightly soluble in water, soluble in alcohol and oils.

Diffusive, penetrating and rather unpleasant odor, in dilution appearing fresh-green with distinct Onion-notes. Solutions in Diethylphthalate of concentration less than 1% have a fresher odor, the "Onion" character being almost imperceptible.

The taste remains, however, Onion-like or slightly Garlic-like at concentrations higher than 2 ppm.

This material has been suggested for use in flavor compositions as a modifier in Onion flavors for meat, sausages, soups, etc.

It represents the typical aroma of the wild "ramson" (Allium ursinum) which is a popular soup ingredient in certain countries, while it has been a folk medicine and also has considerable pharmacological importance in other countries.

The material is not included in the American G.R.A.S. list.

Prod.: from Vinyl chloride plus Potassium sulfide.

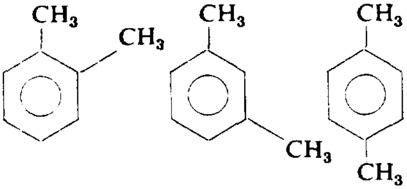
66-348; 96-233;

## 3096: XYLENE

Dimethyl benzene.

$C_8H_{10} = 106.17$

Three isomers are commercially available:



| *ortho*-Xylene. | *meta*-Xylene. | *para*-Xylene. |
|---|---|---|
| Sp.Gr. 0.88 | Sp.Gr. 0.86 | Sp.Gr. 0.86 |
| B.P. 144° C. | B.P. 139° C. | B.P. 138° C. |
| | | M.P. 13° C. |

Colorless liquids.

Insoluble in water, soluble in alcohol and oils. Poorly soluble in diluted alcohol.

Xylene is flammable and its vapors form explosive mixtures with air at room temperature.

Pungent, "gassy", kerosene-like odor, but not nearly as powerful as that of Toluene, not as nauseating as Benzene. Overall sweeter and milder than the two.

Xylene (mixture or isolated isomers) are used as solvents, occasionally for extraction of plant material intended for perfume raw-materials. It is not used as such in perfumes or flavors.

The commercial "Xylene" mixture consists primarily of *meta*-Xylene, with minor amounts of the two other isomers.

Prod.: the commercial "mixture" of isomers is isolated from coal tar from the gasoline fractions.

*ortho*-Xylene, which is the rare isomer, is generally isolated from gasoline, but also produced by pyrolysis of *iso*-Phorone. It finds extensive use in the manufacture of Phthalic anhydride.

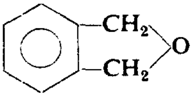
*meta*-Xylene can be produced in a pure state from Toluene sulfonic acid. It is a starting material for the synthesis of Musk Xylene.

*para*-Xylene can be produced pure from *para*-Xylidine.

1-395; 34-806; 68-101; 68-106; 100-1108;
*ortho*-Xylene: B-V-362;
*meta*-Xylene: B-V-370;
*para*-Xylene: B-V-382;

## 3097: ortho-XYLENE OXIDE

*ortho*-Xylyl oxide.
Phthalan.



$C_8H_8O = 120.15$

Colorless liquid. B.P. 190° C.

Very slightly soluble in water, soluble in alcohol and oils.

Heavy, sweet odor of Bitter-Almond-type, but not nearly as pungent as Benzaldehyde, yet not as soft as Tolylaldehyde.

The title material has been suggested for use in perfume compositions, but it is mentioned in this work mostly as a representative of another rare group of materials. The author believes that the title material has little or no application in perfumes or flavors today.

The title oxide also offers some challenge to those interested in studying relationship between chemical structure and olfactory property. Under the title: Catechol methylene ether in this work is mentioned a material of resembling structure and of quite powerful, but not closely related odor.

Prod.: from *ortho*-Xylylene dibromide by heating with Potassium carbonate.

31-150; 68-818;

## 3098: XYLENOL

Hydroxy dimethylbenzene.
Six isomers are known. Five of them are common commercial items.

$C_8H_{10}O = 122.17$

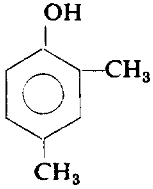
The Xylenols are solid white materials with melting points from 26° up to 75° C. The boiling points vary from 204° C. to 225° C. The specific gravity is slightly higher than 1,00.

They are very slightly soluble in water, soluble in alcohol and oils.

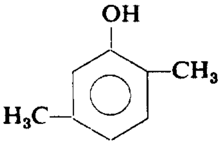
Xylenols are used as disinfectants and bactericides, and as such may be encountered in perfumery as an odor problem to overcome.

The six isomers are briefly mentioned in this work for the sake of elucidating the rather complicated picture, since the word "Xylenol" may be used rather indiscriminately in perfumery literature.

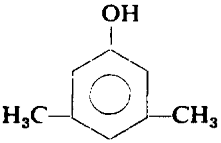
1) *meta-4*-Xylenol.
   Weak odor.
   *2,4*-Xylenol
   *4*-Hydroxy-*1,3*-dimethylbenzene
   *asymmetric-meta*-Xylenol. M.P.26°C.
   Isolated from tar.



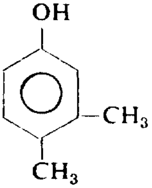
2) *para*-Xylenol.
   Mild, "cresylic" odor.
   *2,5*-Xylenol
   *2*-Hydroxy-*1,4*-dimethylbenzene.
   Isolated from tar.



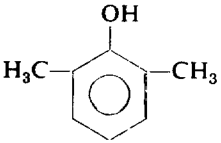
3) *meta-5*-Xylenol.
   Strong, "cresylic" odor.
   *3,5*-Xylenol
   *5*-Hydroxy-*1,3*-dimethylbenzene.
   *symmetric-meta*-Xylenol.
   Isolated from tar, constitutes main portion of tar-Xylenol.



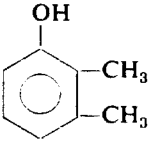
4) *ortho-4*-Xylenol.
   Flat, dry odor.
   *3,4*-Xylenol
   *4*-Hydroxy-*1,2*-dimethylbenzene.
   *asymmetric-ortho*-Xylenol. Isolated from tar.



5) *meta-2*-Xylenol.
   Sweet, "rooty" odor.
   *2,6*-Xylenol
   *2*-Hydroxy-*1,3*-dimethylbenzene.
   *vicinal-meta*-Xylenol.



6) *ortho-3*-Xylenol.
   M.P. 75° C.
   *2,3*-Xylenol
   *3*-Hydroxy-*1,2*-dimethylbenzene.
   *vicinal-ortho*-Xylenol.
   This is the rare isomer of the series.



31-23; 68-420; 100-1109;
B-VI pages:
486(1); 494(2); 492(3);
480(4); 485(5); 480(6);
See also monograph: Cresylic acid.

## 3099: XYLYL ALDEHYDE

Dimethyl benzaldehyde.

Of the six possible isomers, five are relatively well known.

One has been described in this work under the name:

*2,4*-Dimethyl benzaldehyde.

It is, in the author's opinion, the only isomer of any importance to perfumes or flavors.

However, since a product is commercially available under the name Xylyl aldehyde, and since it is apparently an aldehyde derived from mixed isomers of Xylene, not a well-defined, single chemical, it will be briefly mentioned in this work under the title Xylyl aldehyde.

The commercial material is a colorless oily liquid, practically insoluble in water, soluble in alcohol and oils.

B.P. approximately 220° C.

Sweet, mildly floral odor with Bitter-Almond type note.

The title material has been suggested for use in sweet-floral fragrance types, such as Lilac, Appleblossom, etc. Since the *2,4*-Dimethylbenzaldehyde is a commercially available item of reasonable purity, there is probably little chance that the title (mixed isomers) material will become of any importance in future perfumery.

$C_9H_{10}O = 134.18$

The six isomers are:

*2,3*-Dimethyl benzaldehyde

*2,4*-Dimethyl benzaldehyde (mentioned separately in this work)

*2,5*-Dimethyl benzaldehyde

*2,6*-Dimethyl benzaldehyde (rare, not commercially available)

*3,4*-Dimethyl benzaldehyde

*3,5*-Dimethyl benzaldehyde

Most of these materials can be produced by Manganese peroxide oxidation of the corresponding *Tri*methylbenzenes.

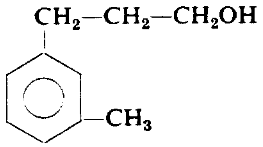
3-127; 68-515; 163-77;

## 3100: beta-meta-XYLYL ETHANOL

*beta-meta*-Xylyl ethylalcohol.

*3*-(*3'*Methylphenyl)-propanol-*1*.

*meta*-Methyl hydrocinnamic alcohol.



$C_{10}H_{14}O = 150.22$

Colorless oily liquid.

Practically insoluble in water, soluble in alcohol and oils.

Mild, sweet-floral, soft-balsamic odor, fresher than Phenylpropylalcohol (Hydrocinnamic alcohol), but less rosy and less balsamic.

The title material has been suggested for use in perfume compositions in general as a mild floralizer or modifier in floral or woody-floral, evt. Oriental-floral compositions.

It blends well with Linalool, Terpineol, "rose alcohols", Cinnamic alcohol etc. in Appleblossom, Lilac, Hyacinth, etc., but it lacks power in proportion to its relatively high cost.

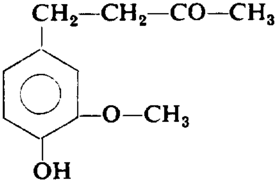
The subject alcohol is rarely offered commercially under its proper chemical name, but may still be used in certain specialties. The author is inclined to believe that the material is obsolete.

Prod.: from *meta*-Methylbenzaldehyde via Perkin's reaction to *meta*-Methylcinnamic acid. The ethylester of this acid is transformed in a Bouveault-Blanc reduction to the title alcohol.

3-172; 4-193; 163-100; 68-500;

# 3101: ZINGERONE

Vanillyl acetone.
*3*-Methoxy-*4*-hydroxy benzylacetone.
*4*-Hydroxy-*3*-methoxy benzylacetone.
*4*-(*3*-Methoxy-*4*-hydroxyphenyl)-*2*-butanone.
(*4*-Hydroxy-*3*-methoxyphenylethyl)-methylketone.
Do not confuse with "Zingiberone".



$C_{11}H_{14}O_3 = 194.23$

Pale yellowish, pale amber-colored or cream-colored crystalline mass. Sp.Gr. 1.14 (liquid). M.P. 41° C. B.P. 290° C.

The once liquefied material will often remain supercooled as a viscous, pale amber-colored liquid at room temperature for a considerable length of time.

Sweet-spicy, warm, heavy-floral, mildly animal-balsamic and Vanilla-like odor with excellent tenacity.

Sweet and spicy, balsamic Vanilla-like taste in concentrations below 40 ppm. Slightly pungent-burning at higher concentrations, but not very pleasant above 100 ppm. The pleasant taste level is generally between 10 and 25 ppm., depending upon accompanying flavor materials.

This ketone finds a little use in perfume compositions as a sweetener of warm, slightly spicy-tobacco-like effect, which can be modified into "leather"-notes, "tabac"-notes or even heavy floral (Jasmin) notes, according to the supplementing fragrance materials. It has often a very attractive influence upon Castoreum and Labdanum, and it blends very well with Ylang and Gardenia bases.

Being a phenol, it carries similar disadvantages as the parent chemical, Vanillin, but it is normally possible to use the required amounts of Zingerone for a fragrance without risking discoloration of the functional product. The material is not recommended for white soap except in very modest amounts.

The perfumery and flavor literature is particular stubborn in repeating (and quoting from other literature) that Zingerone is the pungent principle of Ginger. It is not so. And Zingerone does not have a conspicuously pungent taste. At least, pungency is not the characteristic feature of the flavor of Zingerone. It is an excellent flavor material, not only for Vanilla imitation, where – again – it gives interesting effects with Castoreum, but it is frequently used in many types of imitation fruit flavor, "root beer", Spice blends, Ginger Ale (although it has very little Ginger-note to offer!!) and in tobacco flavorings.

The normal concentration in finished products is about 5 to 15 ppm.

Fortunately, the more authoritative literature (E. Guenther, vol. V. page 119, and Gildemeister-Treibs, vol. IV, page 493) confirm, that the essential oil of Ginger does not contain Zingerone, while G. Fenaroli (Sostanze Aromatiche Naturali, 1963) reports that – according to Miltitzer Berichte, the Oleoresin of Ginger does contain Zingerone.

However, it remains very questionable if Zingerone is present as such in Ginger rhizome. It is most conceivable that it is present in the shape of condensation products with lower alifatic aldehydes, particularly Hexanal and Heptanal, but also probably Nonanal and Decanal.

The condensation product of Zingerone

with any one of these aldehydes is distinctly pungent to the human taste.

Steam distillation may well decompose the condensation product, thus releasing Hexanal, Heptanal, etc., all identified in Ginger (volatile) oil, while the remaining Zingerone portion of the decomposed product is very poorly distillable with steam, and will not show up in the essential oil.

This theory leaves still some unanswered questions about the Oleoresin, which, according to one source, does contain Zingerone (free). A hydrocarbon extraction should not affect the pungent condensation products, and it is well known that Ginger is pungent. It is also known that Ginger Oleoresin may lose its pungency when treated with aqueous alkali. This explains again a decomposition of the condensation product into aldehydes and non-pungent Zingerone. Besides, Ginger Oleoresin is often made by Acetone-extraction, which cannot be classified as a non-hydrous solvent extraction. One thing can safely be deducted from the above mixture of philosophy and facts: Zingerone is NOT the key to characteristic Ginger flavor or flavor effect.

But it has so many other virtues which make it a very useful perfume and flavor material.

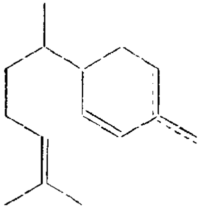
G.R.A.S. F.E.M.A. No.3124.

Prod.: by condensation of Vanillin with Acetone, followed by controlled hydrogenation.

Further hydrogenation (of the ketone group) may yield *4'*(*4*-Hydroxy-*3*-methoxyphenyl)-butan-*2*-ol. That material is known but not commercially available. It has a milder, but similar odor and taste.

1-523; 27-304; 68-755; 100-1119; 103-275; 104-280; 106-350; 140-169; 159-305; 163-77; B-VIII-623, zweiter Ergänzungsband.
See also monograph: Shogaol (2845).

## 3102: ZINGIBERENE



$C_{15}H_{24} = 204.36$

Colorless oily liquid. Sp.Gr. 0.87.
B.P. 270° C.

Practically insoluble in water, soluble in alcohol and oils.

Polymerizes under exposure to air, becomes very viscous, eventually solid and practically odorless.

Freshly prepared material has a warm, woody-spicy and very tenacious odor with a peculiar deep sweetness.

The title sesquiterpene is briefly mentioned in this work, although it is rarely offered commercially, and it has not yet been made by synthesis on a commercial scale. However, since it is the major component of Ginger oil, and the "oxygenated" components of that oil have been found to be rather common and available materials, there could be a future interest in the subject material for reconstitution of Ginger oil if and when it becomes scarce.

Furthermore, the title material has potential interest to the perfumer in its warm-balsamic, almost "Oriental" character, which may remind an observer of Opopanax or Bisabolene. If Zingiberene could be synthesized at a cost below $ 20.— per kilo, it would undoubtedly enter the shelves of scores of perfume laboratories and go far beyond the experimental stage.

For the persons interested in structure and olfactory characteristics, it may be a new field for Sandalwood odor studies, since Zingiberene, after being cyclized to *iso*-Zingiberene becomes a potential intermediate for Sandalwood-smelling chemicals. At the time of editing (Dec. 1968), this idea is, however, of no economical interest.

31-8; 65-87; 87-234; 95-79;

# Tables of odors and flavors, classified in basic groups

To facilitate the locating and tracing of materials of certain commonly used odor (or flavor) type, the following ten tables are included:

*Perfumes:*

1) Ambregris odors
2) "Jasmones" and related materials
3) Musks
4) Pyran derivatives
5) Sandalwood odor chemicals

*Flavors:*

6) Acids (food acids and acid flavors)
7) Bitter flavors
8) Celery aroma chemicals
9) Flavor enhancers, synergists, etc.
10) Food sweeteners or sweetening flavor chemicals.

The above classification is made by unquestionable or conspicuous odor (and flavor) type, NOT by suggested application of a material.

The above tables do therefore NOT include the very large number of other chemicals generally suggested for use in perfume and flavor creations of the said types.

Other tables are included in the monographs of this work as follows:

"Ionones"............ see monograph No.1776

Methylquinolines...... see monograph No.2233

Neo-irones............ see monograph No.2312

Resorcinol ethers...... see monograph No.2796

Thymols.............. see monograph No.2945

Xylenols.............. see monograph No.3098

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*Table No. 1*

AMBREGRIS odor chemicals
(including chemically related materials)

| Monograph No, | |
|---|---|
| 1 | Abietic acid |
| 2 | Abitol |
| 104 | Ambrein |
| 108 | Ambrinol |
| 140 | *alpha-iso*-Amyl-*gamma-n*-butyrolactone |
| 416 | *alpha-n*-Butyl-*gamma*-butyrolactone |
| 594 | *alpha*-Cedrene epoxide |
| 602 | Cedryl formate |
| 701 | Clovene |
| 809 | *gamma*-Cyclo-homogeraniol |
| 823 | Decahydro-*beta*-naphthaldehyde |
| 825 | Decahydro-*beta*-naphthylacetaldehyde |
| 830 | *beta*-Decalone |
| 887 | *2,4*-Di-*tertiary*-butyl-*5*-methoxy benzaldehyde |
| 929 | Dihydro carvyl benzoate |
| 950 | Dihydro-*gamma*-ionone |
| 962 | Dihydro-*delta*-methylionone |
| 1052 | *1,7*-Dimethyl-*4*-*iso*-propylnaphthalene |
| 1053 | *1,6*-Dimethyl-*4*-*iso*-propyl-oxy-decahydronaphthalene |
| 1085 | Di-*iso*-propyl acetophenone |
| 1086 | Di-*iso*-propyl benzaldehyde |
| 1089 | Di-*iso*-propyl dimethyl benzaldehyde |
| 1092 | Di-*iso*-propyl methylbenzaldehyde |
| 1193 | Ethyl citronellyl oxalate |
| 1212 | Ethyl-*2,4*-di-*iso*-propyl phenylglycidate |
| 1213 | *3a*-Ethyl-dodecahydro-*6,6,9a*-trimethylnaphto-(*2,1-b*)-furan |
| 1391 | Fixateur 404 |
| 1589 | Hexahydro tetramethyl naphthalenone |
| 1649 | *alpha-iso*-Hexyl-*gamma-n*-butyrolactone |
| 1791 | Ketone BD-*9* |
| 1835 | Manool |
| 2088 | *beta-iso*-Methylionone |
| 2272 | Mononitro dibromobutyl-*meta*-cresol methylether |
| 2361 | *alpha*-Nonenyl furfuracrolein |
| 2577 | Phenyl naphthyl ketone |
| 2836 | Sclareol |
| 2862 | Squalene |
| 2922 | *5,6,7,8*-Tetrahydro-*1*-(or -*2*-)-naphthylacetaldehyde |
| 2931 | *2,5,5,9*-Tetramethyl-*1*-hydroxy-*1,2,3,5,6,7,8,9*-octahydronaphthalin |
| 2932 | $\Delta^{2,3}$-(and $\Delta^{1,2}$-)-*2,5,5,9*-Tetramethyl octalyl-*1*-ethanal |
| 2933 | $\Delta^{2,3}$-(and $\Delta^{1,2}$-)-*2,5,5,9*-Tetramethyl octalyl-*1*-ethanol |

### *Table No. 2*

## "JASMONES" – and related chemicals

| Monograph No. | |
|---|---|
| 58 | Allethrolone |
| 168 | Amyl cyclopentenone |
| 443 | *2*-Butyl-*2*-cyclopentenone-*1* |
| 954 | Dihydrojasmone |
| 955 | Dihydro-*iso*-jasmone |
| 956 | Dihydro jasmone lactone |
| 1533 | *2-n*-Heptyl cyclopentanol |
| 1534 | *2-n*-Heptyl cyclopentanone |
| 1535 | Heptyl cyclopentenone |
| 1547 | *2-n*-Heptylidene cyclopentanone |
| 1563 | *2*-(*n*-Heptyl)-tetrahydrofuran |
| 1658 | *2*-Hexyl cyclopentanone |
| 1659 | *2-n*-Hexyl-*2*-cyclopenten-*1*-one |
| 1670 | *alpha*-Hexylidene cyclopentanone |
| 1787 | Jasmine lactone |
| 1788 | *cis*-Jasmone |
| 1789 | "*iso*-Jasmone" |
| 1790 | *trans*-Jasmone |
| 1903 | *3*-Methyl-*2*-*iso*-amyl cyclopentanone |
| 1932 | *3*-Methyl-*5*-*n*-butylidene cyclopenten-*2*-one-*1* |
| 2049 | *3*-Methyl-*2*-*n*-heptyl cyclopentan-*1*-one |
| 2064 | Methyl-*3*-hexyl-*2*-cyclopenten-*2*-one-*1* |
| 2076 | Methyl hydrojasmonate |
| 2093 | Methyl jasmonate |
| 2094 | Methyl-*iso*-jasmonate |
| 2420 | *alpha*-Octyl cyclopentanone |
| 2428 | *alpha*-Octylidene cyclopentanone |
| 2457 | *2-n*-Pentylidene cyclohexanone-*1* |
| 2908 | Tetrahydro jasmone |

This table does not include "Jasmin materials" in general.

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### *Table No. 3*

## "MUSKS"

This list includes a few materials which are not exclusively "musk" fragrance materials.

| Monograph No. | |
|---|---|
| 30 | *4*-Acetyl-*6*-*tertiary*-butyl-*1,1*-dimethyl indan |
| 40 | *5*-Acetyl-*1,1,2,3,3,6*-hexamethyl indan |
| 41 | *6*-Acetyl-*1,1,3,4,4,6*-hexamethyl tetrahydro naphthalene |
| 61 | *3-alpha*-Allopregnanol |
| 105 | Ambrettolide |
| 106 | *Δ-5-iso*-Ambrettolide |
| 107 | *Δ-6-iso*-Ambrettolide |
| 140 | *alpha-iso*-Amyl-*gamma-n*-butyrolactone |
| 234 | *3-alpha*-Androstenol |
| 234 | *3-beta*-Androstenol |
| 449 | *3-tertiary*-Butyl-*4*-ethoxy-*5*-nitrobenzaldehyde |
| 468 | *tertiary*-Butylhydroquinone dimethylether |
| 491 | *3-tertiary*-Butyl-*4*-methoy-*5*-nitrobenzaldehyde |
| 555 | Butyryl dinitro-*tertiary*-butyl-*meta*-xylol |
| 608 | *2*-Chloro-*4,6*-dinitro-*1,3*-idmethyl-*5*-*tertiary*-butylbenzene |
| 700 | Civettone |
| 770 | Cyclohexadecane epoxide |
| 771 | Cyclohexadecanone |
| 810 | Cyclopentadecanol |
| 811 | Cyclopentadecanolide |
| 812 | Cyclopentadecanolone |
| 813 | Cyclopentadecanone |
| 816 | Cyclotridecanone |
| 831 | Decamethylene malonate |
| 832 | Decamethylene oxalate |
| 853 | *alpha-n*-Decyl-*gamma*-butyrolactone |
| 881 | *3,5*-Di-*tertiary*-butyl acetophenone |
| 887 | *2,4*-Di-*tertiary*-Butyl-*5*-methoxy benz aldehyde |
| 923 | Dihydro ambrettolide |
| 933 | Dihydro civettone |
| 997 | *3,4*-Dimethyl-*7*-*tertiary*-butyl coumarin |
| 1005 | *1,1*-Dimethyl-*5,7*-di-*iso*-propyl-*6*-indanol |
| 1062 | Dimethyl tetrahydrophenylethyl alcohol |
| 1065 | Dinitro-*tertiary*-butyl pseudo cumene |
| 1066 | Dinitro-*tertiary*-butyl xylene aldehyde |
| 1067 | Dinitro-*tertiary*-butyl xylyl cyanide |
| 1068 | *2,4*-Dinitro-*3*-ethyl-*6*-*tertiary*-butylanisole |
| 1092 | Di-*iso*-propyl methylbenzaldehyde |
| 1094 | *2,4*-Di-*iso*-propyl phenylacetaldehyde |
| 1104 | Dodecamethylene carbonate |
| 1109 | *1,12*-Dodecanolide |
| 1112 | Dodecenyl propionate |
| 1193 | Ethyl citronellyl oxalate |
| 1214 | Ethylene brassylate |
| 1228 | Ethylene undecandioate |
| 1326 | Ethyl pentadecanoate |
| 1392 | *2*-Fluoro-*4,6*-dinitro-*1,3*-dimethyl-*5*-*tertiary*-butylbenzene |
| 1572 | Hexadecamethylenimine |
| 1581 | *1,3,4,6,7,8*-Hexahydro-*4,6,6,7,8,8*-hexamethyl-cyclopenta-*gamma-2*-benzopyran |

| | |
|---|---|
| 1586 | *1,3,4,6,7,8*-Hexahydro-*4,6,6,8,8*-pentamethyl-cyclopenta-*gamma*-*2*-benzopyran |
| 1587 | *3,4,6,7,8,9*-Hexahydro-*4,6,6,9,9*-pentamethyl-*1H*-naphtho-(*2,3c*)-pyran |
| 1591 | Hexamethylene carboxylate |
| 1649 | *alpha*-*iso*-Hexyl-*gamma*-*n*-butyrolactone |
| 1755 | *14*-Hydroxy-*13*-methyl-*1*-tetradecanoic acid, lactone |
| 1758 | *14*-Hydroxy-*4*-oxy-tetradecyl lactone |
| 1982 | *1*-Methyl cyclopentadecan-*2*-one |
| 1983 | *4*-Methyl cyclopentadecanone-*1* |
| 1984 | *5*-Methyl cyclopentadecanone-*1* |
| 1985 | *3*-Methyl cyclopentadecenone |
| 1993 | *4*-Methyl cyclotetradecan-*1*-one |
| 2101 | *1*-Methyl-*3*-methoxy-*4,6*-di-*tertiary*-butyl-*2,5*-dinitrobenzene |
| 2272 | Monitro dibromobutyl-*meta*-cresol methylether |
| 2275 | Moskene |
| 2276 | Muscone |
| 2277 | Muscopyridine |
| 2278 | Musk ambrette |
| 2279 | Musk ketone |
| 2280 | Musk ketone – methylanthranilate |
| 2281 | Musk tibetene |
| 2282 | Musk xylol |
| 2414 | *alpha*-Octyl-*gamma*-butyrolactone |
| 2443 | *10*-Oxahexadecanolide |
| 2444 | *11*-Oxahexadecanolide |
| 2445 | *12*-Oxahexadecanolide |
| 2894 | Tetradecamethylene carboxylate |
| 2983 | Tridecamethylene carboxylate |
| 3017 | Trinitro-*tertiary*-butyltoluene |
| 3026 | Undecamethylene carbonate |
| 3027 | Undecamethylene oxalate |
| 3048 | *alpha*-*n*-Undecyl-*gamma*-butyrolactone |
| 3062 | Valeryldinitro-*tertiary*-butyl-*meta*-xylene |
| 3080 | Versalide |

*Table No. 4*

Summary of PYRAN-derivatives

| Monograph No. | |
|---|---|
| 23 | *cis*-Acetonyl-*2*-methyl-*4*-tetrahydro pyran |
| 44 | *3*-Acetyl-*6*-methyl-*2,4*-pyrandione |
| 963 | Dihydro-*4*-(or -*3*)-(*4*-methyl-*3*(or -*2*-) penten-*1*-yl)-*Δ3*-pyran |
| 1581 | *1,3,4,6,7,8*-Hexahydro-*4,6,6,7,8,8*-hexamethyl-cyclopenta-*gamma*-*2*-benzopyran |
| 1586 | *1,3,4,6,7,8*-Hexahydro-*4,6,6,8,8*-pentamethyl-cyclopenta-*gamma*-*2*-benzopyran |
| 1587 | *3,4,6,7,8,9*-Hexahydro-*4,6,6,9,9*-pentamethyl-*1H*-naphtho-(*2,3c*)-pyran |
| 1629 | *cis*-*3*-Hexenyl-tetrahydro-*2*-pyranylether |
| 1858 | Methallyl acetal dihydropyran |
| 1935 | *5*-Methyl-*3*-butyl tetrahydropyran-*4*-yl acetate |
| 2809 | Rose oxide (Rose oxides) |
| 2915 | Tetrahydro-*5*-(*para*-menthan-*7*-ylmethoxy)-pyran |
| 2924 | Tetrahydro-*2*-(phenethoxy)-pyran |
| 2926 | Tetrahydro pyranyl crotonate |
| 2929 | Tetrahydro-*2*-(*para*-tolyloxy)-pyran |
| 3016 | *2,6,6*-Trimethyl-*6*-vinyl tetrahydropyran |

*Table No. 5*

SANDALWOOD fragrance chemicals

| Monograph No. | |
|---|---|
| 223 | *8*-*tertiary*-Amyl-*1*-tetralone |
| 267 | Atlantone |
| 360 | *iso*-Bornyl methoxy cyclohexanol |
| 406 | *8*-*tertiary*-Butyl-*alpha*-benzosuberone |
| 497 | *8*-*tertiary*-Butyl-*5*-methyl-*alpha*-tetralone |
| 535 | *7*-*tertiary*-Butyl-*alpha*-tetralone-*1* |
| 563 | *3*-(*iso*-Camphenyl-*8*)-*2*-methylpropanol-*1* |
| 564 | *3*-(Camphenyl-*8*)-*2*-methylpropen-*3*-al |
| 566 | *3*-(*iso*-Camphyl-*5*)-cyclohexanol |
| 827 | Decahydro-*beta*-naphthylformate |
| 2008 | *3*-Methylene-*4*-bornylbutanol |
| 2105 | *5*-Methyl-*7*-methoxy-*8*-*iso*-propyl-*alpha*-tetralone |
| 2216 | *3*-Methyl-*4*(*4'*-*iso*-propylcyclohexyl)-butanol |
| 2217 | *3*-Methyl-*4*(*4'*-*iso*-propylcyclohexyl)-butan-*2*-one |
| 2219 | *alpha*-Methyl-*para*-*iso*-propyl hexahydro phenylethyl ketone |
| 2816 | Santalal |
| 2817 | *alpha*-Santalene |
| 2818 | *beta*-Santalene |
| 2819 | *alpha*-Santalol |
| 2820 | *beta*-Santalol |
| 2833 | Santene |
| 2834 | Santenone |
| 3009 | *alpha*-*3,3*-Trimethyl-*2*-norbornane methanol |
| 3012 | *1,1,2*-Trimethyl tetralone-*3* |

### *Table No. 6*

## ACIDS (Food acids and acid flavors)

| Monograph No. | |
|---|---|
| 16 | Acetic acid |
| 266 | Ascorbic acid |
| 380 | Butter acids |
| 549 | *n*-Butyric acid |
| 550 | *iso*-Butyric acid |
| 657 | Citric acid |
| 772 | Cyclohexane acetic acid |
| 775 | Cyclohexane sulfamic acid |
| 1130 | Erythorbic acid |
| 1410 | Formic acid |
| 1411 | Fumaric acid |
| 1418 | *2*-Furoic acid |
| 1596 | Hexanoic acid |
| 1792 | Lactic acid |
| 1798 | Levulinic acid |
| 1829 | *l*-Malic acid |
| 1862 | Methoxy acetic acid |
| 1941 | *alpha*-Methyl butyric acid |
| 2400 | Octanoic acid |
| 2612 | Phosphoric acid |
| 2654 | Propionic acid |
| 2785 | Pyruvic acid |
| 2858 | Sorbic acid |
| 2872 | Tartaric acid |
| 3056 | *n*-Valeric acid |
| 3057 | *iso*-Valeric acid |

### *Table No. 7*

## BITTER flavors

| Monograph No. | |
|---|---|
| 304 | Benzyl diethyl-(*2* : *6*-xylyl-carbamoyl-methyl)-ammonium benzoate |
| 558 | Caffeine |
| 1465 | Glucose penta-acetate |
| 2309 | Naringin |
| 2787 | Quinine |
| 2788 | Quinine bisulfate |
| 2789 | Quinine hydrochloride |
| 2790 | Quinine sulfate |
| 2868 | Sucrose octa-acetate |

This list includes one material which is NOT mentioned in the American G.R.A.S. list (304).

### *Table No. 8*

## CELERY aroma chemicals

| Monograph No. | |
|---|---|
| 473 | *3*-*iso*-Butylidene-*3a*,*4*-dihydrophthalide |
| 475 | *3*-*n*-Butylidene phthalide |
| 476 | *3*-*iso*-Butylidene phthalide |
| 517 | *3*-*n*-Butyl phthalide |
| 925 | Dihydro-*n*-butylidene phthalide |
| 1024 | *alpha*-*beta*-Dimethyl-*gamma*-hydroxy-*gamma*-*n*-butyl-*2*-butenolide |
| 1987 | Methyl cyclopentenolone |
| 2013 | *4*-Methyl-*7*-ethoxy coumarin |
| 2215 | *3*-Methyl-*5*-propyl-*2*-cyclohexenone |
| 2720 | *3*-Propylidene phthalide |
| 2838 | Sedanoic anhydride |
| 2839 | Sedanolic acid |
| 2840 | Sedanolide |
| 2841 | Sedanonic acid |
| 2843 | *beta*-Selinene |
| 3054 | Valeraldehyde diamylacetal |
| 3063 | *3*-*iso*-Validene-*3a*,*4*-dihydrophthalide |
| 3064 | *3*-*iso*-Validene phthalide |
| 3079 | Verbenone |

This list includes a few materials which are not related to the typical Celery natural component chemicals or to the conventional "key" aroma chemicals in Celery flavor.

### *Table No. 9*

## Food FLAVOR ENHANCERS-synergists, etc.

| Monograph No. | |
|---|---|
| 907 | Diethyl glutamate |
| 1097 | Disodium guanylate |
| 1098 | Disodium inosinate |
| 1155 | Ethyl asparaginate |
| 1466 | *laevo*-Glutamic acid |
| 1745 | *3*-Hydroxy-*2*-ethyl-*4*-pyrone |
| 1771 | Ibotenic acid |
| 1831 | Maltol |
| 1899 | *alpha*-Methyl-*alpha*-aminobutyric acid |
| 2245 | *3*-Methyl thiopropyl alcohol |
| 2273 | Monosodium glutamate |
| 2274 | Monosodium-*l*-homocysteinate |
| 2979 | Tricholomic acid |

*Table No. 10*

## Food SWEETENERS or distinctly sweet flavors

| Monograph No. | |
|---|---|
| 112 | *2*-Amino-*4*-nitro-*1*-*n*-propoxybenzene |
| 116 | Ammonium saccharin |
| 146 | *n*-Amyl chloro malonamide |
| 315 | *syn*-*5*-Benzyl-*2*-furfuraldoxime |
| 559 | Calcium acetate |
| 560 | Calcium cyclamate |
| 561 | Calcium saccharin |
| 609 | Chloroform |
| 775 | Cyclohexane sulfamic acid |
| 938 | Dihydro cuminyl aldehyde-anti-aldoxim |
| 1125 | Dulcin |
| 1464 | Glucose |
| 1467 | Glycerin |
| 1471 | Glycyrrhizin, ammoniated |
| 1745 | *3*-Hydroxy-*2*-ethyl-*4*-pyrone |
| 1793 | Lactose |
| 2168 | *N*-Methyl phenethyl carbamide |
| 2310 | Naringin dihydrochalcone |
| 2311 | Neohesperidin dihydrochalcone |
| 2696 | Propylene glycol |
| 2812 | Saccharin |
| 2844 | Serine |
| 2853 | Sodium cyclamate |
| 2857 | Sodium saccharin |

NOTE: This list includes certain materials which are banned from use in food, and also a few materials which have not yet been cleared as G.R.A.S. by the American authorities.

# Explanation to index

This work describes approximately 3,350 chemicals in 3,102 individual monographs. Most of these chemicals are sold under or known under several names, trade names, old erroneous names, misleading chemical names, etc.

In order to improve the usefulness of this work, a cross-index has been included in the back of volume No. Two.

The cross-index has 10,000 names, including the 3,102 monograph title names.

All materials (monographs) have a number assigned to them. Monograph title names are printed in BOLD type in the book, following the monograph number. *Monograph title numbers* are listed in the cross index in the *left hand side* column, and the numbers are consecutive in accordance with the alphabetic listing of the monograph title names.

The synonyms are listed alphabetically in the cross-index with the proper monograph reference number in the column of numbers near the names – the right hand side column of numbers.

The monograph title name may or may not be the correct chemical name for the material in question. In many cases, it has been practical and reasonable to prefer a commercial name, or a very well-known common name, rather than a complicated, hard-to-remember, correct chemical name as title name.

Coumarin, Heliotropine, Cyclamen aldehyde, Vanillin, Citronellol, Geraniol, Eugenol, Maltol, etc. are thus used as head names, since their chemical names are not used in labelling commercial lots of these materials for perfume or flavor use.

However, the use of complicated chemical names for materials, also known under simple trade names, is sometimes preferred in this work. This system offers the advantage of listing together – or near one another – chemically related materials, often with similar olfactory or organoleptic properties.

While it is common in Europe to write Benzyl dimethyl carbinol, it is more common in the U.S.A. to write: Dimethyl benzyl carbinol. The cross-index will always provide the "other" name.

According to modern practice of chemical nomenclature, the monograph title names in this work will generally make use of the rule: "Lowest Alkyl First" – e.g. ETHYL HEPTYL ETHER is title name, while Heptyl ethyl ether becomes its synonym.

In accordance with indexing conventions generally agreed upon, the following prefixes *have been alphabetized:*

ALLO-
ANTI-
CYCLO-
DI-
ENDO-
EPI-
EXO-
HOMO-
MONO-
NEO-
NOR-
TRI-
PSEUDO-

while the following prefixes are NOT *counted for alphabetizing:*

*alpha-* *beta-* *gamma-* *delta-* *omega-* *asymmetric-*
*n-* *iso-* *secondary-* *tertiary-* *primary-* *symmetric-*
*ortho-* *meta-* *para-* *cis-* *trans-* *gem.-*
*bis-* *lin.-* *meso-* *laevo-* *dextro-* *vicinal-*
*dl-* *racemic-* *N-* *O-* *H-* *1, 2, 3,* etc.

Greek prefixes will normally precede numbers in the alphabetic sequence.

All letters NOT counted in the alphabet are written in *script.*

All letters counted in the alphabet are written with CAPITAL LETTERS (in monograph title names) or Gothic type (synonyms).

In order to abbreviate the voluminous index of this work the repetition of certain radicles has been omitted, and the reader is kindly asked to search for synonym radicles in case the synonym he has in mind is not specifically listed.

As an example, METHYL PHENYL CARBINYL CAPRYLATE could be listed under 27 synonyms if the author had made complete use of all the alcohol radicle synonyms and all the acid radicle synonyms for that material. With an average of 28 names per material, we would find about 90,000 names in the index, and it would no longer serve a purpose of time-saving.

The chemical language of most perfumers may be rather confusing to the educated chemist, just as well as the chemist's language is not always appreciated by the perfumer. The author of this work has had to find a reasonably "happy medium" of Aroma-chemical language.

Many chemists prefer to use the name "*para*-Tolyl acetate" for the material which is known to the perfumer as "*para*-Cresyl acetate", while the perfumer uses the name "*para*-Tolyl acetate" for the chemical which is most often "*para*-Methyl benzyl acetate", distinctly different from *para*-Cresyl acetate.

The author has therefore declined from using the radicle "*para*-Tolyl" as a synonym for the "*para*-Cresyl" series of perfume chemicals. Other examples would be parallel to this.

The use of *strict alphabetic order* (same as in the book "Perfume and Flavor Materials of Natural Origin", 1961) may be slightly confusing to some readers in that e.g. a series of "Phenyl*ethyl* ... esters" may be interrupted by one material: Phenyleth*ylidene* acetone – followed by more esters of Phenyl*ethyl* ..., but the author insists on *strict* alphabetic order.

# Radicle synonym list

| | *see also:* |
|---|---|
| -methanoate | -formate |
| -ethanoate | -acetate |
| -propanoate | -propionate |
| -butanoate | -butyrate |
| -pentanoate | -valerate |
| -pentanoate | -valerianate |
| -hexanoate | -caproate |
| -hexanoate | -hexoate |
| -hexanoate | -capronate |
| -hexanoate | -hexylate |
| -heptanoate | -heptoate |
| -heptanoate | -heptylate |
| -octanoate | -octoate |
| -octanoate | -octylate |
| -octanoate | -caprylate |
| -nonanoate | -nonylate |
| -nonanoate | -pelargonate |
| -decanoate | -decylate |
| -decanoate | -caprinate |
| -decanoate | -caprate |
| -undecanoate | -hendecanoate |
| -undecanoate | -undecylate |
| -dodecanoate | -laurate |
| -dodecanoate | -dodecylate |
| -dodecanoate | -laurinate |
| -tetradecanoate | -tetradecylate |
| -tetradecanoate | -myristate |
| -anisate | -*para*-methoxybenzoate |
| -salicylate | -*ortho*-hydroxybenzoate |
| -anthranilate | -*ortho*-aminobenzoate |
| -phenylacetate | -*alpha*-toluate |
| -phenylpropionate | -hydrocinnamate |
| Benzene | Benzol |
| Glycerin | Glycerol |
| Pyrocatechin | Pyrocatechol |
| Pyrocatechin | Catechol |
| Toluene | Toluol |
| Xylene | Xylol |
| Acetals | see name of *parent* aldehyde first |
| *2-* | *ortho-* |
| *3-* | *meta-* |
| *4-* | *para-* |
| *dl-* | *racemic-* |
| Amyl- | Pentyl- |

| | *see also:* |
|---|---|
| Oenanthylidene- | Heptylidene- |
| Capryl- | Octyl- |
| Pelargonyl- | Nonyl- |
| Hendecyl- | Undecyl- |
| Lauryl- | Dodecyl- |
| Myristyl- | Tetradecyl- |
| Cetyl- | Hexadecyl- |
| Allyl- | *2*-Propenyl- |
| Allyl- | Vinyl carbinyl- |
| Cyclohexyl- | Cyclohexan(yl)- |
| Cyclohexyl- | Hexahydrophenyl- |
| Ethenyl- | Vinyl- |
| Ethinyl- | Ethynyl- |
| *iso*-Butenyl- | 2-Methylpropenyl |
| Methylol- | Hydroxymethyl- |
| Thiohydroxy- | Mercapto- |
| Thionyl- | Sulfinyl- |
| Anisal- | Anisylidene- |
| Anisyl- | *para*-Methoxybenzyl- (NOTE: "Chemical Abstracts" include the synonym Methoxyphenyl-, but the author prefers to exclude that synonym from perfumery language). |
| Benzal- | Benzylidene- |
| Benzylcarbinyl- | Phenylethyl- or: Phenethyl- |
| Cinnamal- | Cinnamylidene- (aldehyde) |
| Cinnamenyl- | Styryl- |
| Cresoxy- | Toloxy- |
| Carvacryl- | *2-para*-Cymyl- |
| Guaiacyl- | *ortho*-Methoxyphenyl- |
| Hydrocinnamyl- | Phenylpropyl- |
| Furfural- | Furfurylidene- |
| Salicyl- | *ortho*-Hydroxybenzyl- (NOTE: "Chemical Abstracts" include the synonym *ortho*-Hydroxyphenyl-, but that synonym is not commonly used in perfumery language). |
| *alpha*-Toluyl- | Phenylacetyl- |
| *alpha*-Tolyl- | Benzyl- |
| Vanillal- | Vanillylidene- |
| Heliotropyl- | Piperonyl- |
| Heliotropylidene- | Piperonal- |

# Index

1892 Abalyn
1 .... Abietic acid
1892 Abietic acid, methyl ester
2 .... Abitol
2976 "Abracador"
2350 "Abricolin"
149 A.c.a.
244 "Acaciol"
2273 "Accent"
6 Acetal
3 .... Acetaldehyde
4 .... Acetaldehyde benzyl-*beta*-methoxy acetal
685 Acetaldehyde citronellyl methyl acetal
5 .... Acetaldehyde di-*iso*-amylacetal
6 .... Acetaldehyde diethyl acetal
7 .... Acetaldehyde di-*cis-3*-hexenyl acetal
8 Acetaldehyde-*1,5*-dihydroxypentane acetal
8 .... Acetaldehyde di-Pentanediol acetal
2511 Acetaldehyde di-phenylethyl acetal
9 .... Acetaldehyde di-propyl acetal
682 Acetaldehyde ethyl citronellyl acetal
1195 Acetaldehyde ethyl-*para*-cresyl acetal
10 .... Acetaldehyde ethyl-*trans-3*-hexenyl acetal
1337 Acetaldehyde ethyl phenylethyl acetal
1371 Acetaldehyde eugenyl methyl acetal
685 Acetaldehyde methyl citronellyl acetal
8 Acetaldehyde pentamethyleneglycol acetal
11 Acetaldehyde-*1*-phenyl-*1,2*-ethanediol acetal
11 .... Acetaldehyde phenylethyleneglycol acetal
12 .... Acetaldehyde phenylethyl-*n*-propyl acetal
12 Acetaldehyde-*n*-propyl phenylethyl acetal
12 Acetal R
13 .... Acetanisole
1513 Acetate C-7
2408 Acetate C-8
2363 Acetate C-9
848 Acetate C-10
3041 Acetate C-11, unsaturated
1113 Acetate C-12
2988 Acetate C-13
2451 Acetate C-15
559 Acetate of Lime
91 Acetate P.A.
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15 .... Acet-*iso*-eugenol
16 .... Acetic acid
21 Acetic acid, nitrile
3 Acetic aldehyde
1137 Acetic ether
2271 Acetin
2971 Acetin
3082 Acetivenol
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43 Acetoin
34 Acetol
35 Acetol acetate
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2123 *alpha*-Acetonaphthylene
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19 Acetone diethyl acetal
19 .... Acetone diethyl ketal
20 Acetone dimethyl acetal
20 .... Acetone dimethyl ketal
1468 Acetone glycerol
1893 "Acetone substitute"
21 .... Acetonitrile
22 .... Acetonyl acetone
23 .... *cis*-Acetonyl-*3*-methyl-*4*-tetrahydropyran
2809 *cis*-Acetonyl-*3*-methyl-*4*-tetrahydropyran
24 .... Acetophenone
25 Acetophenone diethyl acetal
25 .... Acetophenone diethyl ketal
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28 .... Acetovanillone
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2771 "Acetylated Citronellal"
24 Acetyl benzene
109 *1*-Acetyl-*2*-aminobenzene
24 Acetyl benzol
2483 Acetyl biphenyl
30 .... *4*-Acetyl-*6*-*tertiary*-butyl-*1,1*-dimethyl indan
31 .... Acetyl-*n*-butyryl
32 .... Acetyl-*iso*-butyryl
33 .... Acetyl caproyl
34 .... Acetyl carbinol
35 .... Acetyl carbinyl acetate
724 Acetyl-*meta*-cresol
2955 Acetyl-*ortho*-cresol

725 Acetyl-*para*-cresol
2077 *5*-Acetyl-*para*-cresol
17 *para*-Acetyl cumene
17 *para*-Acetyl cumol
36 .... Acetyl cyclohexane
37 .... Acetyl cyclohexanol
38 .... *3*-Acetyl cyclopentanone
2211 *2*-Acetyl-*para*-cymene
881 *1*-Acetyl-*3,5*-di-*tertiary*-butylbenzene
30 *4*-Acetyl-*1,1*-dimethyl-*6*-*tertiary*-butyl indan
1000 *3*-Acetyl-*1,1*-dimethyl-*3*-cyclohexene
977 *2*-Acetyl dimethylhydroquinone
2643 Acetylene carbinol
14 Acetyl eugenol
15 Acetyl-*iso*-eugenol
2786 Acetyl formaldehyde
2785 Acetyl formic acid
39 .... Acetyl furan
1475 Acetyl guaiacol
40 .... *5*-Acetyl-*1,1,2,3,3,6*-hexamethyl indan
41 .... *6*-Acetyl-*1,1,3,4,4,6*-hexamethyl tetrahydro naphthalene
1748 *ortho*-Acetylhydroquinone monomethylether
1832 *2*-Acetyl-*3*-hydroxyfuran
42 .... Acetyl mesitylene
1895 *1*-Acetyl-*4*-methylbenzene
1896 *2*-Acetyl-*1*-methyl cyclopentane
43 .... Acetyl methyl carbinol
44 .... *3*-Acetyl-*6*-methyl-*2,4*-pyrandione
27 Acetyl-*2*-methylquinoline
3023 Acetyl nonanoyl
3023 Acetyl nonyryl
3023 Acetyl pelargonyl
47 Acetyl pentanoyl
48 Acetyl-*iso*-pentanoyl
1134 *ortho*-Acetyl phenethole
2491 Acetyl phenol
1723 *2*-Acetyl phenol
1724 *4*-Acetyl phenol
1897 *5*-Acetyl-*2*-picoline
1798 *3*-Acetyl propionic acid
45 .... Acetyl propionyl
17 *1,4*-Acetyl-*iso*-propyl benzol
46 .... *3*-Acetyl pyridine
1747 *4*-Acetylresorcinol monomethylether
3080 *7*-Acetyl-*1,1,4,4*-tetramethyl-*7*-ethyl-*1,2,3,4*-tetralin
1895 *4*-Acetyl toluene
2972 Acetyl tributyl citrate
42 Acetyl-*1,3,5*-trimethylbenzene
47 .... Acetyl valeryl
48 .... Acetyl-*iso*-valeryl
49 .... Acetyl vanillin
3071 Acetylvanillin diacetate
50 .... Acetylvanillin dimethylacetal
978 *4*-Acetyl veratrole
983 Acetyl-*meta*-xylene
51 Achilleic acid
51 .... Aconitic acid
52 Acraldehyde
52 .... Acrolein
52 Acrylaldehyde
53 .... Acrylic acid
52 Acrylic aldehyde
54 .... Adipic acid
2659 Adipic acid, di-*iso*-propylester
814 Adipic ketone
3014 "Adoxal"
1323 Aethon
55 .... Agropyrene
2273 "Ajinomoto"
56 "Alantcamphor"
56 .... Alantolactone
56 *iso*-Alantolactone
2660 Albacol
1144 Alcohol
1597 Alcohol C-6
1501 Alcohol C-7
2401 Alcohol C-8
2348 Alcohol C-9
841 Alcohol C-10
3039 Alcohol C-11, undecylenic
3031 Alcohol C-11, undecylic
1108 Alcohol C-12, lauric
2986 Alcohol C-13
2289 Alcohol C-14
2450 Alcohol C-15
1574 Alcohol C-16
2392 Alcohol C-18
758 Aldehyde B
1592 Aldehyde C-6
1494 Aldehyde C-7
2397 Aldehyde C-8
1257 Aldehyde "*iso*-C-8"
2343 Aldehyde C-9
833 Aldehyde C-10
1031 "*iso*-Aldehyde C-10"
3028 Aldehyde C-11, saturated
3035 Aldehyde C-11, unsaturated
1105 Aldehyde C-12, lauric
2984 Aldehyde C-13
2290 Aldehyde C-14, true
3024 "Aldehyde C-14", so-called
182 "Aldehyde *iso*-C-14"
2261 "Aldehyde *iso*-C-14"
2449 Aldehyde C-15, true
1573 Aldehyde C-16, true
1306 "Aldehyde C-16", so-called
1307 "Aldehyde C-17", so-called
2391 Aldehyde C-18, true
2350 "Aldehyde C-18", so-called
71 "Aldehyde C-19", so-called
293 "Aldehyde C-19", so-called
294 "Aldehyde C-19", Pineapple
1307 "Aldehyde C-20", so-called
2398 Aldehyde C-8, diethyl acetal
3029 Aldehyde C-11, diethyl acetal
3037 Aldehyde C-11, unsaturated, diethyl acetal
2399 Aldehyde C-8, dimethyl acetal
2345 Aldehyde C-9, dimethyl acetal
3030 Aldehyde C-11, dimethyl acetal
1106 Aldehyde C-12, dimethyl acetal
2132 Aldehyde C-12, M.N.A.
256 "Aldehyde Foin Coupe"
256 "Aldehyde F.K."
2145 Aldehyde M.O.A.

1066 Aldehydmoskus
57 .... *4*-Aldehydo phenyl thiocarbimide
57 *para*-Aldehydo phenyl-*iso*-thiocyanate
1534 Alismone
2479 "Alleglal"
2315 "Allerol"
58 .... Allethrolone
2651 Allicin
617 Allo-cinnamic acid
1737 Allofixine
1411 Allo-maleic acid
1832 Allo-maltol
59 .... Allo-ocimene
60 .... Allo-ocimene dioxide
1030 Allo-ocimenol
61 .... *3-alpha*-Allopregnanol
62 .... *Δ-17,20*-Allopregnen-*2*-one
2976 "Allorosol"
63 .... Allyl acetate
2452 Allyl acetic acid
2453 Allyl acetonitrile
64 Allyl-*ortho*-aminobenzoate
84 Allyl amylacetylene carboxylate
393 *alpha*-Allyl-*iso*-amylalcohol
1131 *para*-Allyl anisole
64 .... Allyl anthranilate
65 .... Allyl benzoate
66 .... Allyl benzyl ether
66 Allyl benzyl oxide
393 Allyl-*iso*-butyl carbinol
67 .... Allyl butyrate
68 .... *alpha*-Allyl-*gamma*-Butyrolactone
69 .... Allyl caprate
70 .... Allyl caproate
71 .... Allyl caprylate
80 Allyl-*iso*-caprylate
2453 Allyl carbinyl cyanide
746 Allyl carbinyl-*iso*-thiocyanate
1369 *4*-Allylcatechol-*2*-methylether
1219 Allyl cellosolve
72 .... Allyl cinnamate
73 .... Allyl cyanide
86 Allyl cyclocitrylidene acetone
74 .... Allyl cyclohexane acetate
75 .... Allyl cyclohexane butyrate
76 .... Allyl cyclohexane caproate
78 Allyl cyclohexane pentanoate
77 .... Allyl cyclohexane propionate
78 .... Allyl cyclohexane valerate
74 Allyl cyclohexyl acetate
75 Allyl cyclohexyl-*n*-butyrate
76 Allyl cyclohexyl hexoate
77 Allyl cyclohexyl propionate
78 Allyl-*beta*-cyclohexyl valerianate
3019 *3*-Allyl decahydro-*alpha*-naphthalone
3018 *3*-Allyl decahydro-*alpha*-naphthol
261 *1*-Allyl-*2,5*-dimethoxy-*3,4*-methylenedioxybenzene
874 Allyl disulfide
875 Allyl ether
80 Allyl ethyl butyl acetate
79 .... Allyl-*2*-ethylbutyrate
80 Allyl ethyl caproate
80 .... Allyl-*2*-ethylhexoate
81 .... Allyl formate
82 .... Allyl fumarate
83 Allyl furan-*2*-carboxylate
83 .... Allyl-*2*-furoate
1219 Allyl glycol (mono-)
1369 *4*-Allyl guaiacol (see also 1473)
347 *5*-Allyl guaiacol (see also 1473)
14 Allyl guaiacol acetate
80 Allyl heptane-*gamma*-carboxylate
85 Allyl heptanoate
84 .... Allyl heptin carbonate
84 Allyl heptin carboxylate
85 .... Allyl heptoate
85 Allyl heptylate
97 Allyl-*2,4*-hexadienoate
74 Allyl hexahydro phenylacetate
75 Allyl hexahydro phenylbutyrate
76 Allyl hexyhydro phenylcaproate
77 Allyl hexahydro phenylpropionate
78 Allyl hexahydro phenylvalerianate
70 Allyl-*n*-hexoate
58 *dl-2*-Allyl-*4*-hydroxy-*3*-methyl-*2*-cyclopenten-*1*-one
86 .... Allyl Ionone
86 Allyl-*alpha*-ionone
95 *2*-Allyl-*para*-menthen-*4*-(*8*)-one-*3*
87 .... Allyl mercaptan
2291 *4*-Allyl-*6*-methoxy-*1,2*-methylenedioxybenzene
1369 *4*-Allyl-*2*-methoxyphenol
14 *4*-Allyl-*2*-methoxyphenyl acetate
284 *4*-Allyl-*2*-methoxyphenyl benzoate
1373 *4*-Allyl-*2*-methoxyphenyl formate
99 Allyl-*trans-2*-methyl-*2*-butenoate
2813 *4*-Allyl-*1,2*-methylenedioxybenzene
98 Allyl mustard oil
88 .... Allyl nonanoate
89 Allyl nonenoate
88 Allyl nonylate
89 .... Allyl-*2*-nonylenate
71 Allyl octoate
84 Allyl-*2*-octynoate
85 Allyl oenanthate
103 *3*-Allyl-oxy-*4*-hydroxy benzaldehyde
88 Allyl pelargonate
90 .... *para*-Allyl phenethole
606 *para*-Allyl phenol
91 .... Allyl phenoxy acetate
92 .... Allyl phenylacetate
72 Allyl-*beta*-phenylacrylate
2497 Allyl phenylether
93 .... Allyl propionate
94 .... Allyl propyl disulfide
95 .... Allyl pulegone
2813 *meta*-Allyl pyrocatechin methylene ether
98 Allyl-*iso*-rhodanide
96 .... Allyl salicylate
98 Allyl senevol
97 .... Allyl sorbate
87 Allyl sulfhydrate
876 Allyl sulfide
98 Allyl-*iso*-sulfocyanate
98 Allyl thiocarbimide
98 .... Allyl-*iso*-thiocyanate

87 Allyl thiol
99 .... Allyl tiglate
99 Allyl tiglinate
1127 *4*-Allyl-*1,2,6*-trimethoxybenzene
101 Allyl-*10*-undecenoate
100 .... Allyl undecylate
101 .... Allyl undecylenate
102 Allyl valerate
102 .... Allyl-*iso*-valerate
102 Allyl-*iso*-valerianate
103 .... Allyl vanillin
2026 *4*-Allyl veratrole
1039 *para*-Allyl-*meta*-xylenol
1833 "Almond water, Bitter"
387 "Alpha-isopropyl muguetton"
758 "Alpine violet"
268 "Amandiol"
268 "Amandol"
2867 "Amber acid"
2132 "Ambra-aldehyde"
887 "Ambral"
104 .... Ambrein
104 Ambreinolide
2278 Ambrette moskus
105 .... Ambrettolide
106 .... Δ-*5*-*iso*-Ambrettolide
107 .... Δ-*6*-*iso*-Ambrettolide
1193 "Ambrettozon"
108 .... Ambrinol
1086 Ambriol
2132 Ambrolene
3035 "Ambrolione"
109 .... *ortho*-Amino acetophenone
240 Aminobenzene
401 *ortho*-Amino-*iso*-butylbenzoate
110 .... *alpha*-Aminobutyric acid
111 .... *alpha*-Amino-*iso*-butyric acid
1154 *2*-Amino ethylbenzoate
1641 *ortho*-Amino-*n*-hexylbenzoate
2939 *2*-Amino-*3*-hydroxybutanoic acid
2939 *alpha*-Amino-*beta*-hydroxybutyric acid
2844 *alpha*-Amino-*beta*-hydroxypropionic acid
1910 *ortho*-Amino methylbenzoate
1899 *dl*-*2*-Amino-*2*-methylbutanoic acid
3065 *2*-Amino-*3*-methylbutanoic acid
112 .... *2*-Amino-*4*-nitro-*1*-*n*-propoxybenzene
128 *iso*-Aminopentane
1466 *2*-Aminopentane dioic acid
240 Aminophen
1466 *1*-Aminopropane-*1,3*-dicarboxylic acid
3065 *alpha*-Amino-*iso*-valeric acid
115 Ammonia solution
115 "Ammonia spirit"
115 Ammonia water
116 Ammonium-*ortho*-benzsulfinimide
113 Ammonium bicarbonate
113 Ammonium carbamate
113 .... Ammonium carbonate
114 .... Ammonium chloride
1471 Ammonium glycyrrhizate
115 .... Ammonium hydroxide
116 .... Ammonium saccharin
117 .... Ammonium sulfide
118 Ammonium valerate
118 .... Ammonium-*iso*-valerate
118 Ammonium-*iso*-valerianate
119 Amyl acetate
119 *dextro*-Amyl acetate
119 .... *iso*-Amyl acetate
119 *normal*-Amyl acetate
120 .... *secondary*-*n*-Amyl acetate
121 .... *tertiary*-Amyl acetate
122 .... "*tertiary*"-Amyl acetate, so-called
123 .... *iso*-Amyl acetoacetate
192 *iso*-Amyl acetopropionate
124 .... *alpha*-Amyl acrolein
125 .... *n*-Amyl alcohol
126 .... *iso*-Amyl alcohol
1424 *iso*-Amyl alcohol
127 .... *secondary*-*n*-Amyl alcohol
1008 *tertiary*-Amyl alcohol
3052 Amyl aldehyde
3053 *iso*-Amyl aldehyde
128 .... *iso*-Amyl amine
129 .... *iso*-Amyl angelate
130 .... Amyl anisate
130 *iso*-Amyl anisate
131 .... Amyl anthranilate
131 *iso*-Amyl anthranilate
132 .... Amyl benzoate
132 *iso*-Amyl benzoate
133 .... *iso*-Amyl benzyl acetate
134 .... Amyl benzyl carbinol
135 .... *iso*-Amyl benzyl ether
135 *iso*-Amyl benzyl oxide
136 .... Amyl butyrate
137 Amyl butyrate
137 .... *iso*-Amyl butyrate
138 .... *iso*-Amyl-*iso*-butyrate
139 .... *secondary*-*n*-Amyl butyrate
140 .... *alpha*-*iso*-Amyl-*gamma*-*n*-butyrolactone
2350 *gamma*-*n*-Amyl butyrolactone
2142 *gamma*-*iso*-Amyl butyrolactone
141 .... Amyl caprate
141 *iso*-Amyl caprinate
142 .... Amyl caproate
143 .... *iso*-Amyl caproate
144 .... Amyl caprylate
145 Amyl caprylate
145 .... *iso*-Amyl caprylate
145 *iso*-Amyl-*n*-caprylate
1597 *n*-Amyl carbinol
146 .... *n*-Amyl chloro malonamide
149 Amylcinnamal
150 *iso*-Amylcinnamal
154 *alpha*-*n*-Amylcinnamal diethyl acetal
155 *alpha*-*n*-Amylcinnamal dimethyl acetal
147 Amyl cinnamate
147 .... *iso*-Amyl cinnamate
148 .... Amyl cinnamic alcohol
149 .... Amyl cinnamic aldehyde
150 .... *alpha*-*iso*-Amyl cinnamic aldehyde
151 .... *alpha*-Amyl cinnamic aldehyde diamyl acetal

152 .... *alpha*-Amyl cinnamic aldehyde dibutyl acetal
153 .... Amyl cinnamic aldehyde di-cinnamyl acetal
154 .... Amyl cinnamic aldehyde diethyl acetal
155 .... Amyl cinnamic aldehyde dimethyl acetal
156 .... *alpha*-Amyl cinnamic aldehyde-di-(*iso*)-propyl acetal
157 .... *alpha*-Amyl cinnamic aldehyde-Methylanthranilate
158 .... Amyl cinnamyl acetate
148 Amyl cinnamyl alcohol
159 .... Amyl cinnamyl formate
160 .... *alpha*-Amyl cinnamyl nitrile
161 .... Amyl cinnamyl-*iso*-valerate
162 .... Amyl citrate
1906 Amyl-*meta*-cresotinate
709 "Amyl cresyl oxide"
232 "Amyl crotonyl acetate"
160 *alpha*-Amyl-*alpha*-cyanostyrene
163 .... Amyl cyclohexane acetate
164 .... Amyl cyclohexane propionate
165 .... *para-tertiary*-Amyl cyclohexanol
166 .... *para-tertiary*-Amyl cyclohexanone
167 .... *ortho-tertiary*-Amyl cyclohexyl acetate
2076 *2*-Amyl cyclopentanoneacetic acid, methylester
168 .... Amyl cyclopentenone
168 *2-n*-Amyl cyclopenten-*2*-one-*1*
168 *iso*-Amyl cyclopentenone
148 Amyl dihydrocinnamyl alcohol
129 *iso*-Amyl-*cis-2,3*-dimethyl acrylate
225 *iso*-Amyl-*trans-alpha-beta*-dimethyl acrylate
191 *iso*-Amyl dodecylate
196 Amyl-*alpha-beta*-epoxy methylacetate
169 .... Amyl ether
169 *iso*-Amyl ether
170 .... Amyl eugenol
171 .... Amyl-*iso*-eugenol
172 .... Amyl formate
173 .... *iso*-Amyl formate
174 .... *iso*-Amyl-*2*-furan butyrate
177 *iso*-Amyl-*2*-furancrotonate
175 .... *iso*-Amyl-*2*-furan propionate
174 Amyl furfhydracrylate
176 .... *alpha*-Amyl furfur acrolein
175 "*iso*-Amyl furfurhydracrylate"
175 *alpha-iso*-Amyl furfuryl acetate
177 .... *iso*-Amyl furfuryl acrylate
175 *iso*-Amyl furfuryl propionate
174 *alpha-iso*-Amyl furfuryl propionate
178 .... Amyl furoate
179 .... *iso*-Amyl furoate
179 *iso*-Amyl-*2*-furoate
176 *alpha*-Amyl-*beta-2*-furyl acraldehyde
176 *alpha*-Amyl furylacrolein
177 *iso*-Amyl-*beta*-furyl acrylate
180 .... *iso*-Amyl geranate
183 Amyl heptanoate
184 *iso*-Amyl-*n*-heptanoate
181 .... *iso*-Amyl heptin carbonate
181 *iso*-Amyl heptin carboxylate
182 .... Amyl heptyl acetaldehyde
183 .... Amyl heptylate
184 .... *iso*-Amyl heptylate
185 Amyl heptyl ether
185 .... *iso*-Amyl heptyl ether
185 *iso*-Amyl heptyl oxide
163 Amyl hexahydro phenylacetate
164 Amyl hexahydro phenylpropionate
143 *iso*-Amyl-*n*-hexoate
143 "Amyl hexylate"
142 *n*-Amyl-*n*-hexylate
204 *iso*-Amyl hexynoate
186 .... *alpha*-Amyl hydrocinnamic alcohol
187 .... *alpha*-Amyl hydrocinnamic aldehyde
230 *iso*-Amyl-*4*-hydroxy-*3*-methoxybenzoate
1906 Amyl-*2*-hydroxy-*para*-toluate
3055 *iso*-Amylidene phenylglycol acetal
188 .... *2*-Amyl-*5*-(*or-6*-)keto-*1,4*-dioxane
877 Amyl ketone
189 .... *iso*-Amyl ketone
192 *iso*-Amyl-*gamma*-ketovalerate
190 .... Amyl lactate
190 *iso*-Amyl lactate
191 Amyl laurate
191 .... *iso*-Amyl laurate
192 *iso*-Amyl laevulate
192 .... Amyl levulinate
193 .... Amyl malonate
194 .... Amyl mercaptan
224 Amyl mercapto acetate
195 .... *iso*-Amyl methacrylate
130 *iso*-Amyl-*para*-methoxybenzoate
195 *iso*-Amyl-*alpha*-methylacrylate
129 *iso*-Amyl-*cis-2*-methylcrotonate
196 .... Amyl methyl glycidate
1150 Amyl methyl glycidic acid, ethylester
1905 Amyl methyl ketone
1906 Amyl-*para*-methylsalicylate
197 .... Amyl myristate
197 *iso*-Amyl myristate
198 Amyl nitrate
198 .... *iso*-Amyl nitrate
199 "Amyl nitrite"
199 .... *iso*-Amyl nitrite
200 *iso*-Amyl nonanoate
149 Amyl nonenal
1548 *2*-Amyl nonenal
200 .... *iso*-Amyl nonylate
201 *iso*-Amyl nonynoate
220 Amyl octadecanoate
219 *iso*-Amyl-*1,8*-octane dicarboxylate
144 Amyl octanoate
145 *iso*-Amyl octanoate
201 .... *iso*-Amyl octin carbonate
201 *iso*-Amyl-*n*-oct-*1*-yne carboxylate
181 *iso*-Amyl octynoate
183 "Amyl oenanthate"
202 .... Amyl oleate
202 *iso*-Amyl oleate
203 .... Amyl oxalate
169 *iso*-Amyl oxide
170 "Amyl oxyeugenol"
171 "Amyl oxy-*iso*-eugenol"
200 *iso*-Amyl pelargonate

204 .... *iso*-Amyl-*n*-pentin carbonate
204 *iso*-Amyl-*n*-pent-*1*-yne carboxylate
205 Amyl phenol
205 .... *para-tertiary*-Amyl phenol
206 .... *para-tertiary*-Amyl phenoxy acetaldehyde
207 .... *para-tertiary*-Amyl acetaldehyde diethyl acetal
208 Amyl phenylacetate
208 .... *iso* Amyl phenylacetate
158 *alpha-n*-Amyl-*beta*-phenylacryl acetate
147 *iso*-Amyl-*beta*-phenylacrylate
159 *alpha-n*-Amyl-*beta*-phenylacryl formate
161 *alpha-n*-Amyl-*beta*-phenylacryl-*iso*-valerate
133 *alpha-iso*-Amyl phenyl carbinyl acetate
209 *1*-(*4-tertiary*-Amylphenyl)-ethanol
134 *alpha*-Amyl phenylethyl alcohol
209 .... *para-tertiary*-Amyl phenylethyl alcohol
210 "Amyl phenylethyl ether"
210 .... *iso*-Amyl phenylethyl ether
211 .... Amyl phenyl ketone
186 *alpha-n*-Amyl phenylpropanol
187 *alpha*-Amyl phenylpropionic aldehyde
187 *alpha-n*-Amyl phenyl propyl aldehyde
212 .... Amyl phthalate
2143 *beta*-Amylpropenoic acid, methyl-ester
213 .... *iso*-Amyl propionate
214 .... *alpha*-Amyl-*para-iso*-propyl cinnamic aldehyde
215 .... *alpha-iso*-Amyl pyridine
215 *2-iso*-Amyl pyridine
216 *4*-Amyl pyridine
216 .... *gamma*-Amyl pyridine
178 Amyl pyromucate
179 *iso*-Amyl pyromucate
217 *iso*-Amyl pyroracemate
217 .... *iso*-Amyl pyruvate
218 Amyl salicylate
218 .... *iso*-Amyl salicylate
219 .... *iso*-Amyl sebacate
220 .... Amyl stearate
220 *iso*-Amyl stearate
221 .... *iso*-Amyl succinate
222 .... Amyl tartrate
223 *8-tertiary*-Amyl-*alpha*-tetrahydronaphthalone
223 .... *8-tertiary*-Amyl-*1*-tetralone
194 Amyl thioalcohol
224 .... Amyl thioglycolate
225 .... *iso*-Amyl tiglate
208 *iso*-Amyl-*alpha*-toluate
226 .... *iso*-Amyl undecylate
227 .... *iso*-Amyl undecylenate
228 .... Amyl valerate
228 *n*-Amyl-*n*-valerate
229 *iso*-Amyl valerianate
229 .... *iso*-Amyl-*iso*-valerate
229 *iso*-Amyl-*iso*-valerianate
829 Amyl-*delta*-valerolactone
230 .... *iso*-Amyl vanillate
231 .... Amyl vinyl carbinol
232 .... Amyl vinyl carbinyl acetate
233 .... Amyl vinyl carbinyl propionate
1687 Androl
234 .... *3-alpha*-Androstenol
234 .... *3-beta*-Androstenol
235 .... Δ*1-16*-Androstenone-*3*
2359 "Andryl acetate"
236 .... Anethole
236 *cis*-Anethole
1131 *iso*-Anethole
236 *trans*-Anethole
237 .... Anethole mercaptan
238 .... Angelic acid
129 Angelic acid, *iso*-amylester
239 .... Angelica lactone
811 Angelica lactone, so-called
2336 Aniba canellila oil
240 .... Aniline
241 Anisal
256 Anisalacetone
249 Anisalcohol
241 .... Anisaldehyde
1864 *iso*-Anisaldehyde
1864 *ortho*-Anisaldehyde
241 *para*-Anisaldehyde
242 .... Anisaldehyde diethyl acetal
243 .... Anisaldehyde dimethyl acetal
244 .... Anisaldehyde-Methylanthranilate
236 "Anise camphor"
245 .... Anisic acid
245 *para*-Anisic acid
249 Anisic alcohol
241 Anisic aldehyde
1883 Anisic ketone
1883 Anisketone
246 .... Anisole
1882 "*para*-Anisyl acetaldehyde"
247 .... Anisyl acetate
1865 "*iso*-Anisyl acetate"
248 .... Anisyl acetone
1883 *para*-Anisyl acetone
249 .... Anisyl alcohol
250 .... Anisyl benzoate
251 .... Anisyl benzyl diketone
252 .... Anisyl butyrate
253 .... Anisyl-*iso*-butyrate
254 .... Anisyl formate
255 .... Anisyl heptoate
256 .... Anisylidene acetone
1907 Anisylidene methyl ethyl ketone
257 .... Anisylidene Thujone
1883 Anisyl methyl ketone (see also 13)
258 .... Anisyl phenylacetate
259 .... Anisyl propionate
260 .... Anisyl valerate
260 Anisyl-*iso*-valerate
2650 *para*-Anol
913 Anozol
510 "Anther"
1728 "Anthosal"
1735 "Anthralal"

2124 Anthralone (see also 2123)
1768 Antioxidant (for perfume solutions)
2945 "Antioxine"
1853 "Antisolaire"
60 A.O.D.
261 .... Apiole
262 .... *iso*-Apiole
28 Apocynin
1829 "Apple acid"
1130 *D*-Arabascorbic acid
2819 "Argeol"
2819 "Arheol"
1223 "Arosol"
263 .... Artemisia ketone
1857 "Artemisial"
264 .... Asarone
292 Ascabiol
265 .... Ascaridole
266 .... Ascorbic acid
1130 *iso*-Ascorbic acid
266 *laevo*-Ascorbic acid
2858 Ash, Mountain
2853 Assugrin
1214 "Astrotone"
267 .... Atlantone
241 "Aubepine"
241 "Aubepine liquid"
13 Aubepinol
13 Aubepinone
1735 "Auralva"
1735 "Aurangeol"
2135 "Auranil M.N.A."
1735 "Auranol"
1735 "Aurantine"
1735 "Aurantiol" (see also 1433)
1735 "Auriol"
2733 Australol
2732 Australol ethylether
572 A-vitamin (Provitamin A)
1051 Avolin
2255 Ayapanin
2792 *2*-Azanaphthalene
2783 Azole

B

2637 "Baking powder"
496 "Bamca"
706 Beechwood creosote
2293 Benihinal
292 Benylate
318 Benzal acetone
319 Benzal acetophenone
268 .... Benzaldehyde
1833 Benzaldehyde cyanohydrin
273 Benzaldehyde cyclic acetal of Glycerin
269 .... Benzaldehyde diethyl acetal
270 .... Benzaldehyde-di-(ethyleneglycol monobutylether)-acetal
271 .... Benzaldehyde dimethyl acetal
272 .... Benzaldehyde ethyleneglycol acetal
273 .... Benzaldehyde glyceryl acetal
274 .... Benzaldehyde propyleneglycol acetal
273 "Benzalglycerin"
2791 *1*-Benzaline
321 Benzal mesityloxide
2792 *2*-Benzazine
1772 *1*-Benzazole
278 Benzene
268 Benzene carbonal
276 Benzene carboxylic acid
2793 *1,3*-Benzene diol
268 Benzene methylal
2579 Benzene propionic acid
2937 Benzene thiol
2501 Benzenyl-*ortho*-aminothiophenol
275 .... Benzhydrol
934 *1,2*-Benzodihydropyrone
276 .... Benzoic acid
279 Benzoic acid, nitrile
268 Benzoic aldehyde
277 .... Benzoin
278 .... Benzol
279 .... Benzonitrile
280 .... Benzophenone
2791 *2,3*-Benzopyridine
2792 *3,4*-Benzopyridine
704 *1,2*-Benzopyrone
704 *5,6*-Benzo-*alpha*-pyrone
1772 Benzopyrrole
281 .... Benzoquinone
281 *ortho*-Benzoquinone
282 .... *para*-Benzoquinone
1476 "Benzosol"
2812 *ortho*-Benzosulfimide
1161 Benzoyl acetic ester
283 .... Benzoyl acetone
280 Benzoyl benzene
284 .... Benzoyl eugenol
285 .... Benzoyl-*iso*-eugenol
1476 Benzoyl guaiacol
24 Benzoyl methide
277 *dl*-Benzoyl phenylcarbinol
1765 *beta*-Benzoxy propionaldehyde diethyl acetal
1763 *beta*-Benzoxy propionic aldehyde
1772 *2,3*-Benzpyrrole
2812 *1,2*-Benz-*iso*-thiazol-*3*-(*2H*)-one-*1,1*-dioxide
2580 Benzyl acetaldehyde
286 .... Benzyl acetate
2579 Benzyl acetic acid
287 .... Benzyl aceto acetate
288 .... Benzyl acetone
289 .... Benzyl acetophenone
287 Benzyl acetyl acetate
290 .... Benzyl alcohol
66 Benzyl allyl ether
66 Benzyl allyl oxide
291 Benzyl-*ortho*-aminobenzoate
134 Benzyl amyl alcohol
407 Benzyl-*iso*-amyl alcohol
899 *alpha*-Benzyl-*secondary*-amylalcohol
135 Benzyl-*iso*-amyl ether
135 Benzyl-*iso*-amyl oxide
291 .... Benzyl anthranilate
1080 Benzyl benzene
292 Benzyl benzene carboxylate
292 .... Benzyl benzoate
333 *para*-Benzyl benzylcyanide
293 Benzyl-*n*-butanoate
301 Benzyl-*trans*-*2*-butenoate

2669 Benzyl butyl alcohol
407 Benzyl-*iso*-butyl carbinol
408 Benzyl-*iso*-butyl carbinyl acetate
409 Benzyl butylether
410 Benzyl-*iso*-butylether
2201 Benzyl-*iso*-butyl ketone
410 Benzyl-*iso*-butyl oxide
293 .... Benzyl butyrate
294 .... Benzyl *iso*-butyrate
295 .... *alpha*-Benzyl-*gamma*-butyrolactone
296 .... Benzyl caprate
297 .... Benzyl caproate
298 .... Benzyl caprylate
2513 Benzyl carbinol
2512 Benzyl carbinyl acetate
2514 Benzyl carbinyl anthranilate
2522 Benzyl carbinyl cinnamate
2537 Benzyl carbinyl ethyl methyl acetate
2529 Benzyl carbinyl formate
2539 Benzyl carbinyl-*alpha*-furan-carboxylate
2518 Benzyl carbinyl hexylate
2533 Benzyl carbinyl-*alpha*-hydroxypropionate
2535 Benzyl carbinyl-*alpha*-methylacrylate
2547 Benzyl carbinyl nonylate
2519 Benzyl carbinyl octylate
2548 Benzyl carbinyl phenylacetate
2549 Benzyl carbinyl propionate
2551 Benzyl carbinyl salicylate
2555 Benzyl carbinyl tiglate
2557 Benzyl carbinyl valerianate
2558 Benzyl carbinyl-*iso*-valerianate
329 Benzyl chloracetate
299 .... Benzyl cinnamate
300 .... Benzyl citronellol
710 Benzyl-*para*-cresylether
710 Benzyl cresyl oxide
301 .... Benzyl crotonate
301 Benzyl-*alpha*-crotonate
302 .... Benzyl cyanide
296 Benzyl decanoate
296 Benzyl decylate
303 .... Benzyl dichloro acetate
899 Benzyl diethyl carbinol
304 .... Benzyl diethyl (*2*:*6*-xylyl-carbamoyl-methyl)-ammonium benzoate
344 Benzyl-*trans*-*alpha*-*beta*-dimethyl acrylate
989 Benzyl dimethyl carbinol
991 Benzyl dimethyl carbinyl acetate
992 Benzyl dimethyl carbinyl-*n*-butyrate
993 Benzyl dimethyl carbinyl-*iso*-butyrate
305 .... Benzyl-*2*,*3*-dimethyl crotonate
2471 *2*-Benzyl-*4*,*5*-dimethyl-*1*,*3*-dioxolan
2487 *2*-Benzyl-*1*,*3*-dioxolan
306 .... Benzyl dipropyl ketone
307 .... Benzyl disulfide
324 Benzyl dodecanoate
324 Benzyl dodecylate
879 Benzyl ether
308 .... Benzyl ethoxy acetate
2589 Benzyl ethyl alcohol
1164 Benzyl-*N*-ethyl anthranilate
309 .... Benzyl ethyl butyrolactone
310 .... Benzyl ethylcaproate
1166 Benzyl ethyl carbinol
1167 Benzyl ethyl carbinyl acetate
1168 Benzyl ethyl ether
310 Benzyl-*2*-ethylhexanoate t
310 Benzyl ethyl hexylate
2016 Benzyl ethyl methyl carbinol
2017 Benzyl ethyl methyl carbinyl acetate
311 .... Benzyl eugenol
312 .... *cis*-Benzyl-*iso*-eugenol
313 .... *trans*-Benzyl-*iso*-eugenol
314 .... Benzyl formate
315 .... *syn*-*5*-Benzyl-*2*-furfuraldoxime
317 Benzyl heptanoate
148 *2*-Benzyl-*7*-heptanol
306 *3*-Benzyl-*4*-heptanone
316 .... Benzyl heptin carbonate
317 .... Benzyl heptoate
317 Benzyl heptylate
1520 Benzyl heptyl ether
1520 "Benzyl heptyl oxide"
297 Benzyl hexanoate
297 Benzyl hexoate
297 Benzyl hexylate
1644 Benzyl hexyl ether
1644 Benzyl hexyl oxide
340 Benzyl-*ortho*-hydroxybenzoate
318 .... Benzylidene acetone
2171 Benzylidene acetone methyl
319 .... Benzylidene acetophenone
320 .... Benzylidene crotonaldehyde
273 *1*,*2*-Benzylidene glycerol
273 *1*,*3*-Benzylidene glycerol
149 *2*-Benzylidene heptanal
318 "Benzylidene ketone"
321 .... Benzylidene mesityloxide
1911 Benzylidene-*para*-methyl acetophenone
2171 Benzylidene methyl ethyl ketone
322 .... *alpha*-Benzylidene propiophenone
323 .... *beta*-Benzyl indole
323 *3*-Benzyl indole
880 Benzyl ketone
324 .... Benzyl laurate
325 .... Benzyl mercaptan
343 Benzyl mercaptoacetate
326 .... Benzyl methacrylate
4 Benzyl methoxymethyl acetal
327 .... *2*-Benzyl-*4*-methoxymethyl-*1*,*3*-dioxolan
313 Benzyl-*2*-methoxy-*4*-propenyl phenylether
328 .... Benzyl methyl acetone
326 Benzyl-*alpha*-methylacrylate
301 Benzyl-*beta*-methylacrylate
346 Benzyl-*3*-methylbutyrate
1917 Benzyl methyl carbinol
1918 Benzyl methyl carbinyl acetate
344 Benzyl-*trans*-*alpha*-methylcrotonate
1919 Benzyl methyl ether
2016 Benzyl methyl ethyl carbinol
2017 Benzyl methyl ethyl carbinyl acetate
1920 Benzyl methyl ketone
294 Benzyl-*2*-methyl propanoate
305 Benzyl methyl tiglate

329 .... Benzyl monochloro acetate
342 "Benzyl mustard oil"
330 .... Benzyl myristate
2297 Benzyl-*beta*-naphthyl ether
331 Benzyl nonanoate
331 Benzyl nonylate
298 Benzyl octanoate
298 Benzyl octoate
298 Benzyl octylate
879 Benzyl oxide
4 *1*-Benzyloxy-*1*-(*beta*-methoxy)-ethoxyethane
331 .... Benzyl pelargonate
345 Benzyl-*n*-pentanoate
346 Benzyl-*iso*-pentanoate
135 Benzyl-*iso*-pentyl ether
332 .... Benzyl phenylacetate
333 .... *para*-Benzyl phenylacetonitrile
299 Benzyl-*beta*-phenylacrylate
334 .... Benzyl phenyl carbinol
335 .... Benzyl phenyl carbinyl acetate
2490 *2*-Benzyl-*4*-phenyl-*1,3*-dioxolan
336 .... Benzyl phenyl ether
337 .... Benzyl phenylethyl ether
292 Benzyl phenyl formate
336 Benzyl phenyl oxide
338 Benzyl propanoate
2071 *beta*-Benzylpropanol-*1*
326 Benzylpropen-*1*-carboxylate
338 .... Benzyl propionate
991 Benzyl-*iso*-propylacetate
989 *alpha*-Benzyl-*iso*-propylalcohol
2669 Benzyl-*n*-propylcarbinol
2670 Benzyl-*iso*-propylcarbinol
2671 Benzyl-*iso*-propylcarbinyl acetate
2673 Benzyl-*n*-propyl ether
2674 Benzyl-*iso*-propyl ether
995 Benzyl-*iso*-propyl propionate
339 .... *2*-Benzyl pyridine
339 *alpha*-Benzyl pyridine
340 .... Benzyl salicylate
341 .... Benzyl succinate
330 Benzyl tetradecanoate
342 .... Benzyl-*iso*-thiocyanate
343 .... Benzyl thioglycolate
325 Benzyl thiol
344 .... Benzyl tiglate
332 Benzyl-*alpha*-toluate
2170 Benzyl tolyl ether
2483 *2*-Benzyl-*4,4,6*-trimethyl-*meta*-dioxan
345 .... Benzyl valerate
346 .... Benzyl-*iso*-valerate
345 Benzyl valerianate
347 .... Betelphenol
872 Biacetyl
1576 Biallyl
824 Bicyclo-*4:4:0*-decanol
2387 Bicyclo-(*2:2:1*)-hepta-*2,5*-diene
942 Bicyclo-(*2:2:1*)-heptanol
943 Bicyclo-(*2:2:1*)-heptanyl acetate
942 Bicyclo-(*2:2:1*)-hept-*5*-ene-*2*-aldehyde
942 Bicyclo-(*2:2:1*)-hept-*5*-ene-*2*-aldehyde dimethyl acetal
817 Bicyclo heptenylacetate
818 Bicyclo heptenyl ethylcarbonate
789 *ortho*-Bicyclohexanone
790 *para*-Bicyclohexanone
3081 Bicyclo vetiverol
1735 "Bigariol"
1077 Biphenyl
878 Biphenylene oxide
2241 Birch, sweet (synthetic oil of)
348 .... Bisabolene
348 *gamma*-Bisabolene
349 .... Bisabolol
349 *alpha*-Bisabolol
304 "Bitrex THS-839"
268 "Bitter Almond oil, synthetic"
1833 "Bitter Almond Water"
2332 Bois de Rose oil (see also 2336)
1411 Boletic acid
350 Borneo camphor
350 .... *dextro*-Borneol
351 .... *laevo*-Borneol
352 .... *iso*-Borneol
353 "Bornyl acetate"
353 .... *laevo*-Bornyl acetate
354 .... *iso*-Bornyl acetate
350 Bornyl alcohol
355 .... *iso*-Bornyl benzoate
356 .... Bornyl butyrate
357 Bornyl butyrate
356 *laevo*-Bornyl-*n*-butyrate
357 *laevo*-Bornyl-*iso*-butyrate
357 .... *iso*-Bornyl-*iso*-Butyrate
358 .... Bornyl formate
358 *laevo*-Bornyl formate
359 .... *iso*-Bornyl formate
360 .... *iso*-Bornyl methoxy cyclohexanol
361 .... Bornyl phenylacetate
361 *laevo*-Bornyl phenylacetate
362 .... Bornyl propionate
362 *laevo*-Bornyl propionate
363 .... *iso*-Bornyl propionate
364 .... *iso*-Bornyl salicylate
364 *dextro*-Bornyl salicylate
365 .... Bornyl valerate
366 .... Bornyl-*iso*-valerate
365 *laevo*-Bornyl-*n*-valerate
366 *dextro*-Bornyl-*iso*-valerate
367 .... *iso*-Bornyl valerate
367 *dextro*-*iso*-Bornyl-*n*-valerate
368 .... *iso*-Bornyl-*iso*-valerate
1363 "Bourbonal"
1364 "*iso*-Bourbonal"
1024 "Bovolide"
1012 "Brazinol"
1013 "Brazinyl acetate"
1014 "Brazinyl-*iso*-butyrate"
1015 "Brazinyl formate"
1016 "Brazinyl propionate"
1741 Brevifolin
2301 "Bromelia"
369 .... Bromo ethylbenzene
2272 *4*-Bromo-*3*-methyl-*6*-*tertiary*-butylanisole
371 *1*-Bromo-*2*-phenylethylene
370 *alpha*-Bromostyrene
371 *beta*-Bromostyrene

371 *omega*-Bromostyrene
370 .... *alpha*-Bromostyrol
371 .... *omega*-Bromostyrol
1069 "Buchu camphor"
496 Bucinal
1799 Bucinal-methylanthranilate
547 *n*-Butanal
372 .... Butane
372 *iso*-Butane
1941 Butane-*2*-carboxylic acid
54 *1,4*-Butane dicarboxylic acid
2867 Butane dioic acid
448 *1,3*-Butanediol
373 .... *1,4*-Butanediol di-vinylether
872 *2,3*-Butane dione
488 Butanethiol-*1*
549 *n*-Butanoic acid
389 *1*-Butanol
391 *2*-Butanol
390 *primary-iso*-Butanol
552 *1,2*-Butanolide
552 *1,4*-Butanolide
43 *2*-Butanol-*3*-one
2020 *2*-Butanone
1828 *cis*-Butene dioic acid
1411 *trans*-Butene dioic acid
73 *3*-Butene nitrile
2269 *1*-Buten-*3*-one
73 *beta*-Buteno nitrile
747 *2*-Buten-*1*-yl benzoate
2453 *3*-Butenyl cyanide
374 .... *5*-(or-*2*-)-(*3*-Buten-*2*-yl)-*3*-cyclohexene carboxaldehyde
375 .... *5*-(*3*-Buten-*2*-yl)-*3*-cyclohexene methanol
376 .... *iso*-Butenyl cyclopentanol
748 *2*-Buten-*1*-yl heptanoate
377 .... *beta*-Butenyl-*para*-methoxybenzene
377 *4*-(*2*-Butenyl)-methoxybenzene
378 .... *5*-(*3*-Buten-*2*-yl)-*1*-methyl-*3*-cyclohexene carboxaldehyde
379 .... *alpha*-Butenyl pyridine
379 *2*-(*1*-Butenyl)-pyridine
894 *2*-Butenyl sulfide
746 *beta*-Butenyl-*iso*-thiocyanate
746 *gamma*-Butenyl-*iso*-thiocyanate
749 *2*-Buten-*1*-yl-*alpha*-toluate
470 "Butoben"
997 "Butolia"
514 *iso*-Butoxybenzene
1220 *2*-Butoxyethanol acetate
380 .... Butter acids
1178 Butter ether
381 .... Butter esters
382 .... *n*-Butyl acetate
383 .... *iso*-Butyl acetate
2267 *iso*-Butyl acetic acid
2266 *secondary*-Butyl acetic acid
384 .... Butyl aceto acetate
385 .... *iso*-Butyl aceto acetate
386 .... *para-iso*-Butyl acetophenone
387 .... *para-tertiary*-Butyl acetophenone
483 *n*-Butyl acetopropionate
1506 *beta*-Butyl acrolein
388 .... *iso*-Butyl acrolein
389 .... *n*-Butyl alcohol
390 .... *iso*-Butyl alcohol
391 .... *n*-secondary-Butyl alcohol
392 .... *tertiary*-Butyl alcohol
547 *n*-Butyl aldehyde
548 *iso*-Butyl aldehyde
393 .... *iso*-Butyl allyl carbinol
400 *n*-Butyl-*ortho*-aminobenzoate
401 *iso*-Butyl-*ortho*-aminobenzoate
394 .... *tertiary*-Butyl-*tertiary*-amylketone
395 .... *n*-Butyl angelate
396 .... *iso*-Butyl angelate
490 *meta-tertiary*-Butyl anisaldehyde
397 .... *n*-Butyl anisate
398 .... *iso*-Butyl anisate
399 .... *tertiary*-Butyl anisate
400 .... *n*-Butyl anthranilate
401 .... *iso*-Butyl anthranilate
402 .... *para-tertiary*-Butyl benzaldehyde
411 *para-tertiary*-Butyl benzalacetone
403 .... *n*-Butyl benzoate
404 .... *iso*-Butyl benzoate
406 *8-tertiary*-Butyl-*alpha*-benzocycloheptanone
405 .... *tertiary*-Butyl benzol
406 .... *8-tertiary*-Butyl-*alpha*-benzosuberone
513 *alpha-iso*-Butyl benzylacetate
511 *alpha-n*-Butyl benzylalcohol
512 *alpha-iso*-Butyl benzylalcohol
407 .... *iso*-Butyl benzyl carbinol
408 .... *iso*-Butyl benzyl carbinyl acetate
409 .... Butyl benzyl ether
410 .... *iso*-Butyl benzyl ether
411 .... *para-tertiary*-Butyl benzylidene acetone
409 *n*-Butyl benzyl oxide
410 *iso*-Butyl benzyl oxide
412 *n*-Butyl-*n*-butanoate
414 *iso*-Butyl-*n*-butanoate
412 .... *n*-Butyl-*n*-butyrate
413 .... *n*-Butyl-*iso*-butyrate
414 .... *iso*-Butyl-*n*-butyrate
415 .... *iso*-Butyl-*iso*-butyrate
416 .... *alpha-n*-Butyl-*gamma*-butyrolactone
2403 *gamma-n*-Butyl-*gamma*-butyrolactone
2395 *gamma-iso*-Butyl-*gamma*-butyrolactone
417 .... Butyl butyryl lactate
418 .... Butyl caprate
418 Butyl caprinate
419 .... *n*-Butyl caproate
410 .... *iso*-Butyl caproate
421 .... *n*-Butyl caprylate
422 .... *iso*-Butyl caprylate
431 *tertiary*-Butyl carbimide
125 *n*-Butyl carbinol
126 *iso*-Butyl carbinol
119 *secondary*-Butyl carbinyl acetate
122 *tertiary*-Butyl carbinyl acetate
137 *iso*-Butyl carbinyl butyrate
138 *iso*-Butyl carbinyl-*iso*-butyrate
1936 *d-secondary*-Butyl carbinyl-*iso*-pentanoate
128 *iso*-Butyl carbylamine
1220 Butyl cellosolve acetate

470 "Butyl chemosept"
425 Butyl cinnamal
426 *iso*-Butyl cinnamal
423 .... *n*-Butyl cinnamate
424 .... *iso*-Butyl cinnamate
425 .... *alpha-n*-Butyl cinnamic aldehyde
426 .... *alpha-iso*-Butyl cinnamic aldehyde
427 .... *iso*-Butyl citral
428 .... *n*-Butyl citrate
429 .... *para-tertiary*-Butyl-*meta*-cresol
430 .... *para-tertiary*-Butyl-*meta*-cresol methylether
711 "Butyl cresyl oxide"
492 *beta-tertiary*-Butyl crotonaldehyde
431 .... *tertiary*-Butyl-*iso*-cyanate
466 *n*-Butyl cyclohexane carboxylate
432 .... *ortho-tertiary*-Butyl cyclohexanol
433 .... *para-tertiary*-Butyl cyclohexanol
434 .... *ortho-secondary*-Butylcyclohexanone
435 .... *ortho-tertiary*-Butyl cyclohexanone
436 .... *para-tertiary*-Butyl cyclohexanone
447 *para-tertiary*-Butyl cyclohexene carboxaldehyde (cyclic) Ethyleneglycol acetal
437 .... *iso*-Butyl cyclohexyl acetate
438 .... *ortho-tertiary*-Butyl cyclohexyl acetate
439 .... *para-secondary*-Butyl cyclohexyl acetate
440 .... *para-tertiary*-Butyl cyclohexyl acetate
441 .... *cis-para-tertiary*-Butyl cyclohexyl acetate
442 .... Butyl cyclohexyl caproate
442 *ortho-tertiary*-Butyl cyclohexyl hexanoate
442 *para-tertiary*-Butyl cyclohexyl hexanoate
443 .... *2*-Butyl-*2*-cyclopentenone-*1*
418 Butyl decanoate
444 .... Butyl-*3*-decenoate
418 Butyl decylate
444 *n*-Butyl decylenate
445 .... *iso*-Butyl dihydrocinnamic aldehyde
395 *n*-Butyl-*cis-2,3*-dimethylacrylate
540 *n*-Butyl-*trans-alpha-beta*-dimethylacrylate
396 *iso*-Butyl-*cis-2,3*-dimethylacrylate
997 *tertiary*-Butyl dimethylcoumarin
446 .... *ortho-tertiary*-Butyl-*4,5*-dimethyl phenol
546 *para-tertiary*-Butyl-*meta-3,5*-dimethyl phenol
2279 *4-tertiary*-Butyl-*3,5*-dinitro-*2,6*-dimethyl acetophenone
2281 *5-tertiary*-Butyl-*4,6*-dinitro-hemimellitene
447 .... *8-tertiary*-Butyl-*1,4*-dioxaspiro-*4,5*-decane
482 *n*-Butyl dodecanoate
482 *n*-Butyl dodecylate
448 .... *1,3*-Butylene glycol
448 *beta*-Butylene glycol
391 Butylene hydrate
449 .... *3-tertiary*-Butyl-*4*-ethoxy-*5*-nitrobenzaldehyde
1257 Butyl ethyl acetaldehyde
1503 *n*-Butyl ethyl carbinol
422 *iso*-Butyl-*2*-ethylhexanoate
1173 Butyl ethyl ketone
450 .... Butyl ethyl malonate
1175 "Butyl ethyl malonate"
451 .... *iso*-Butyl everninate
452 .... *n*-Butyl formate
453 .... *iso*-Butyl formate
3057 *iso*-Butylformic acid
454 .... Butyl furacrylate
455 .... *iso*-Butyl furacrylate
454 *n*-Butyl-*beta-2*-furanacrylate
455 *iso*-Butyl-*2*-furanacrylate
454 *n*-Butyl furfuracrylate
455 *iso*-Butyl furfuracrylate
456 .... Butyl furfur hydracrylate
457 "Butyl furfur hydracrylate"
457 .... *iso*-Butyl furfurhydracrylate
458 .... *n*-Butyl furoate
458 *n*-Butyl-*2*-furoate
459 .... *secondary*-Butyl furoate
454 *n*-Butyl-*beta-2*-furylacrylate
455 *iso*-Butyl-*beta-2*-furylacrylate
457 *iso*-Butyl furylpropionate
462 *n*-Butyl heptanoate
463 *iso*-Butyl heptanoate
460 .... *iso*-Butyl heptenone
460 *6-iso*-Butyl-*5*-hepten-*2*-one
461 .... *iso*-Butyl heptin carbonate
462 .... *n*-Butyl heptoate
463 .... *iso*-Butyl heptoate
462 *n*-Butyl heptylate
463 *iso*-Butyl heptylate
464 .... *n*-Butyl heptyl ether
465 .... *iso*-Butyl heptyl ether
465 *iso*-Butyl heptyl oxide
461 *iso*-Butyl hept-*1*-yne-*1*-carboxylate
466 .... Butyl hexahydro benzoate
419 *n*-Butyl hexanoate
420 *iso*-Butyl hexanoate
420 *iso*-Butyl-*n*-hexoate
419 *n*-Butyl hexylate
420 *iso*-Butyl hexylate
467 .... Butyl hexyl ketone
494 *iso*-Butyl-*iso*-hexynoate
515 *iso*-Butyl hydrocinnamate
445 *iso*-Butyl hydrocinnamic aldehyde
468 .... *tertiary*-Butylhydroquinone dimethylether
469 .... Butyl hydroxy anisole
529 *n*-Butyl-*ortho*-hydroxybenzoate
530 *iso*-Butyl-*ortho*-hydroxybenzoate
470 .... Butyl-*para*-hydroxybenzoate
528 *n*-Butyl-*12*-hydroxy-*9*-octadecanoate
882 *4*-Butyl-*4*-hydroxyoctanoic acid, *gamma*-lactone
481 Butyl-*alpha*-hydroxypropionate
471 .... Butyl hydroxy toluene
472 .... Butylidene acetone
473 .... *3-iso*-Butylidene-*3a,4*-dihydrophthalide
474 .... *1,2*-Butylidene dioxypropanol
475 .... *3-n*-Butylidene phthalide
476 .... *3-iso*-Butylidene phthalide

477 .... *alpha-iso*-Butyl indole
477 *2-iso*-Butyl indole
478 .... *beta-iso*-Butyl indole
478 *3-iso*-Butyl indole
479 .... *2*-Butyl-*5*-(or-*6*-)-Keto-*1,4*-Dioxan
480 .... *iso*-Butyl ketone
481 .... *n*-Butyl lactate
483 *n*-Butyl laevulinate (-laevulate)
482 .... *n*-Butyl laurate
483 .... *n*-Butyl levulinate
451 "*iso*-Butyl lichenol"
484 .... *iso*-Butyl linalool
485 .... *iso*-Butyl linalool oxide
486 .... Butyl maleate
487 .... Butyl malonate
1175 Butylmalonic acid, diethylester
1175 "Butyl malonic ester"
488 .... *n*-Butyl mercaptan
539 *n*-Butyl mercaptoacetate
489 .... *n*-Butyl methacrylate
490 .... *3-tertiary*-Butyl-*4*-methoxybenzaldehyde
397 *n*-Butyl-*para*-methoxybenzoate
398 *iso*-Butyl-*para*-methoxybenzoate
399 *tertiary*-Butyl-*para*-methoxybenzoate
491 .... *3-tertiary*-Butyl-*4*-methoxy-*5*-nitrobenzaldehyde
451 *iso*-Butyl-*para*-methoxy orsellinate
430 *4-tertiary*-Butyl-*3*-methoxytoluene
492 .... *beta-tertiary*-Butyl-*beta*-methylacrolein
489 *n*-Butyl-*alpha*-methylacrylate
430 *2-tertiary*-Butyl-*5*-methylanisole
493 .... *iso*-Butyl-*N*-methylanthranilate
395 *n*-Butyl-*cis-2*-methylbutenoate
540 *n*-Butyl-*2*-methyl-*2*-butenoate
396 *iso*-Butyl-*cis-2*-methylbutenoate
494 .... *iso*-Butyl-*3*-methyl-*n*-but-*1*-in carbonate
395 *n*-Butyl-*cis-2*-methylcrotonate
396 *iso*-Butyl-*cis-2*-methylcrotonate
540 *n*-Butyl-*trans-alpha*-methylcrotonate
2278 *6-tertiary*-Butyl-*3*-methyl-*2,4*-dinitroanisole
1930 *iso*-Butyl-*3*-methyl-*2*-furylketone
495 .... *para-iso*-Butyl-*alpha*-methyl hydrocinnamic aldehyde
496 .... *para-tertiary*-Butyl-*alpha*-methyl hydrocinnamic aldehyde
1933 *iso*-Butyl methyl ketone
2618 *tertiary*-Butyl methyl ketone
1934 *para-tertiary*-Butyl methyl phenylacetate
413 *n*-Butyl-*2*-methylpropanoate
415 *iso*-Butyl-*2*-methylpropanoate
497 .... *8-tertiary*-Butyl-*5*-methyl-*alpha*-tetralone
536 "*n*-Butyl mustard oil"
537 "*iso*-Butyl mustard oil"
498 .... *n*-Butyl myristate
499 .... Butyl nicotinate
491 *3-tertiary*-Butyl-*5*-nitroanisic aldehyde
502 *n*-Butyl nonanoate
502 *iso*-Butyl nonanoate
502 *iso*-Butyl nonylate
532 *n*-Butyl octadecanoate
421 *n*-Butyl octanoate
422 *iso*-Butyl octanoate
421 *n*-Butyl octylate
422 *iso*-Butyl octylate
461 *iso*-Butyl octynoate
500 .... *n*-Butyl oleate
501 .... Butyl oxalate
470 "Butyl paraben"
470 "Butyl parasept"
502 *n*-Butyl pelargonate
502 .... *iso*-Butyl pelargonate
503 *iso*-Butyl pentadecanoate
503 .... *iso*-Butyl pentadecylate
3006 *tertiary*-Butyl-*iso*-pentanal
542 *n*-Butyl pentanoate
544 *n*-Butyl-*iso*-pentanoate
543 *iso*-Butyl-*n*-pentanoate
545 *iso*-Butyl-*iso*-pentanoate
3007 *tertiary*-Butyl-*iso*-pentanol
504 Butylphen
504 .... *para-tertiary*-Butyl phenol
505 .... *iso*-Butyl phenoxyacetate
506 .... *para-tertiary*-Butyl phenylacetaldehyde
507 .... *n*-Butyl phenylacetate
508 *ortho-secondahy*-Butyl phenylacetate
508 .... *para-secondary*-Butyl phenylacetate
509 .... *para-tertiary*-Butyl phenylacetate
510 .... *iso*-Butyl phenylacetate
425 *alpha-n*-Butyl-*beta*-phenylacrolein
426 *alpha-iso*-Butyl-*beta*-phenylacrolein
423 *n*-Butyl phenylacrylate
411 *4-(para-tertiary*-Butylphenyl)-*3*-buten-*2*-one
511 .... *n*-Butyl phenyl carbinyl
512 .... *iso*-Butyl phenyl carbinol
513 .... *iso*-Butyl phenyl carbinyl acetate
3055 *2-iso*-Butyl-*4*-phenyl-*meta*-dioxolan
447 *2-(para-tertiary*-Butylphenyl)-*1,3*-dioxolan
514 .... *iso*-Butyl phenylether
408 *alpha-iso*-Butyl phenylethyl acetate
407 *alpha-iso*-Butyl phenylethyl alcohol
3060 Butyl phenyl ketone
3061 *iso*-Butyl phenyl ketone
515 .... *iso*-Butyl phenyl propionate
445 *para-iso*-Butyl-*beta*-phenylpropionic aldehyde
516 *n*-Butyl phthalate
516 .... *iso*-Butyl phthalate
517 .... *3-n*-Butyl phthalide
518 *iso*-Butyl piperonilate
519 .... *iso*-Butyl piperonylate
489 *n*-Butylpropen-*1*-carboxylate
519 .... *n*-Butyl propionate
520 .... *iso*-Butyl propionate
521 .... *iso*-Butyl pyridine
521 *alpha-iso*-Butyl pyridine
521 *gamma-iso*-Butyl pyridine
521 *4-iso*-Butyl pyridine
522 .... *4-tertiary*-Butyl pyridine
522 *gamma-tertiary*-Butyl pyridine
458 *n*-Butyl pyromucate

523 .... *iso*-Butyl quinoline-*2*
524 .... *iso*-Butyl quinoline
523 *alpha-iso*-Butyl quinoline
524 *6-secondary*-Butyl quinoline
525 .... *8-secondary*-Butyl quinoline
525 *ortho-secondary*-Butyl quinoline
526 .... *tertiary*-Butyl quinoline
526 *2-tertiary*-Butyl quinoline
527 .... *para-tertiary*-Butyl resorcinol dimethylether
537 "*iso*-Butyl-*iso*-rhodanide"
538 "*secondary*-Butyl-*iso*-rhodanide"
528 .... Butyl ricinoleate
529 .... *n*-Butyl salicylate
530 .... *iso*-Butyl salicylate
889 *n*-Butyl sebacate
531 .... *tertiary*-Butyl sebacate
532 .... Butyl stearate
411 *para-tertiary*-Butyl styryl methyl ketone
533 .... Butyl succinate
890 *n*-Butyl sulfide
538 *secondary*-Butyl-*iso*-sulfocyanate
534 .... *n*-Butyl tartrate
503 *iso*-Butyl tetradecane-*1*-carboxylate
498 *n*-Butyl tetradecanoate
535 .... *7-tertiary*-Butyl-*alpha*-tetralone-*1*
536 .... *n*-Butyl-*iso*-thiocyanate
537 .... *iso*-Butyl-*iso*-thiocyanate
538 .... *secondary*-Butyl-*iso*-thiocyanate
431 *tertiary*-Butyl-*iso*-thiocyanate
539 .... *n*-Butyl thioglycolate
540 .... *n*-Butyl tiglate
507 *n*-Butyl-*alpha*-toluate
510 *iso*-Butyl-*alpha*-toluate
2281 *5-tertiary*-Butyl-*1,2,3*-trimethyl-*4,6*-dinitrobenzene
3017 *meta-tertiary*-Butyl trinitrotoluene
2282 *5-tertiary*-Butyl-*2,4,6*-trinitro-*meta*-xylene
541 Butyl-*10*-undecenoate
541 .... *n*-Butyl undecylenate
545 Butyl valerate
542 .... *n*-Butyl valerate
543 .... *iso*-Butyl valerate
544 .... Butyl-*iso*-valerate
545 .... *iso*-Butyl-*iso*-valerate
542 *n*-Butyl-*n*-valerianate
544 *n*-Butyl-*iso*-valerianate
2342 *alpha-n*-Butyl-*delta*-valerolactone
546 .... *4-tertiary*-Butyl-*meta-3,5*-xylenol
547 .... *n*-Butyraldehyde
548 .... *iso*-Butyraldehyde
1750 Butyraldol
549 .... *n*-Butyric acid
412 *n*-Butyric acid, *n*-butylester
414 *n*-Butyric acid, *iso*-butylester
550 .... *iso*-Butyric acid
413 *iso*-Butyric acid, *n*-butylester
415 *iso*-Butyric acid, *iso*-butylester
547 *n*-Butyric aldehyde
548 *iso*-Butyric aldehyde
551 .... *iso*-butyric anhydride
1178 Butyric ether
2973 Butyrin
1757 Butyroin
552 .... *gamma-n*-butyrolactone
1090 Butyrone
553 .... Butyrophenone
554 .... Butyryl acetophenone
554 *omega*-Butyryl acetophenone
555 .... Butyryl dinitro-*tertiary*-Butyl-*meta*-xylol
556 .... *iso*-Butyryl formaldehyde
551 *iso*-Butyryl oxide
149 Buxine
148 Buxinol

C

2400 C-8, acid
436 C-64, product
1052 Cadalene
1052 *iso*-Cadalin
557 .... Cadinene
558 .... Caffeine
1800 Cajeputene
616 "Cajeputol"
559 .... Calcium acetate
560 .... Calcium cyclamate
560 Calcium cyclohexane sulfamate
560 Calcium cyclohexyl sulfamate
561 Calcium di-*ortho*-benzosulfimide
2854 Calcium gluconate
2974 Calcium phosphate, dibasic
2974 Calcium phosphate, "*tertiary*"
2974 Calcium phosphate, tribasic
561 .... Calcium saccharin
560 Calcium sucaryl
2854 "Calgon"
2835 "California soap plant"
350 *d*-Camphanol
350 *2*-Camphanol
565 *2*-Camphanone
562 .... Camphene
1028 "Camphene carbinol"
1029 "Camphene carbinyl acetate"
563 *3*-(Camphenyl-*8*)-*2*-methylpropanol-*1*
563 .... *3*-(*iso*-Camphenyl-*8*)-*2*-methylpropanol-*1*
564 .... *3*-(Camphenyl-*8*)-*2*-methylpropen-*3*-al
1943 *trans*-Campholic acid, dimethylester
565 .... *dextro*-Camphor
2813 "Camphor oil 1070"
2813 Camphor oil, "sassafrassy"
566 .... *3*-(*iso*-Camphyl-*5*)-cyclohexanol
566 *meta*-(*iso*-Camphyl-*5*)-cyclohexanol
711 "Cananga ether" (see also 719)
719 "Canangol"
55 Capillen
833 Capraldehyde
835 Capraldehyde-D.m.a.
840 Capric acid
841 Capric alcohol
833 Capric aldehyde
833 Caprinaldehyde
1592 Caproaldehyde
1759 Caproaldol
1596 Caproic acid
2267 *iso*-Caproic acid
1597 Caproic alcohol

1592 Caproic aldehyde
1593 Caproic aldehyde diethyl acetal
1183 Caproic ether
877 Caprone
189 *iso*-Caprone
211 Caprophenone
2404 Caproyl ethanol
735 *para*-Caproyl toluene
2408 Capryl acetate
2401 *n*-Caprylalcohol (see also 2057)
1260 "Capryl alcohol"
2057 *secondary, inactive* Caprylalcohol
2421 Caprylene
2400 Caprylic acid
2040 *iso*-Caprylic acid
2397 Caprylic aldehyde
1257 "*iso*-Caprylic aldehyde"
2059 *iso*-Caprylic formate
2439 Caprylidene
2403 Caprylolactone
2510 Carbanil
567 .... Capsaicine
567 Capsicum (see also 2353 and 2355)
1898 Carbinol
904 "Carbitol" (see also 905)
568 .... Carbon disulfide
1571 Carbon hexachloride
51 *2*-Carboxy glutaconic acid
929 Cardanol (see also 1712)
569 .... Cardanyl benzoate (see also 929 and 1712)
570 .... *Δ3*-Carene and *Δ4*-Carene
2995 "Carene epoxide"
926 Carhydranol (see also 1712)
928 Carhydrine
571 .... Carone
572 .... *beta*-Carotene
1052 Carotol
573 .... Carvacrol
574 .... Carvacryl acetate
575 .... Carvacryl benzoate
576 .... Carvacryl ethylether
577 .... Carvacryl formate
2211 Carvacryl methyl ketone
1800 Carvene
578 .... *laevo*-Carveol
2870 Carvestrene
579 "Carvol"
2876 *4*-Carvomenthenol
579 .... *dextro*-Carvone
580 .... *laevo*-Carvone
581 .... Carvotanacetone
582 .... *laevo*-Carvyl acetate
583 .... *laevo*-Carvyl propionate
1369 Carygenol
1370 *iso*-Carygenol
584 *alpha*-Caryophyllene
584 .... *beta*-Caryophyllene
585 .... Caryophyllene acetate
586 .... Caryophyllene alcohol
586 *beta*-Caryophyllene alcohol
585 Caryophyllene alcohol acetate
1712 Cashew shell oil
619 "Cassia aldehyde"
247 "Cassie ketone" (see also 248)
1488 "Cassione"
587 .... Catechol cyclo-trimethylene ether
883 Catechol dibutyl ketal
884 Catechol di-*iso*-butyl ketal
588 .... Catechol diethylether
3078 Catechol dimethylether
589 .... Catechol di-*n*-propyl ketal
590 .... Catechol di-*iso*-propyl ketal
1473 Catechol methyl allyl ether
1901 Catechol methyl amyl ketal
1927 Catechol methyl butyl ketal
591 .... Catechol methylene ether
1474 Catechol methyl ethyl ether
592 .... Catechol methyl hexyl ketal
1136 Catechol monoethyl ether
1472 Catechol monomethyl ether
2314 Catnip oil
2855 Caustic soda
2096 "Cayenol"
593 .... Cedrene
594 .... *alpha*-Cedrene epoxide
595 .... Cedrenol
596 .... Cedrenone
597 .... Cedrenyl acetate
598 .... Cedrol
599 .... Cedrol methylether
596 "Cedrone"
600 .... Cedryl acetate
601 .... Cedryl cinnamate
602 .... Cedryl formate
603 .... Cedryl phenylacetate
2215 "Celery ketone"*)
30 "Celestolide"
1221 Cellosolve
2980 Celluflex
1728 Centaflor
1043 "Centifol"
1044 "Centifolin"
671 "Cephreine"
669 "Cephrol"
1464 Cerelose
2445 "Cervolide"
2085 "Cetone alpha"
2087 "Cetone beta"
2124 "Cetone D"
86 "Cetone V"
1574 Cetylalcohol
2447 Cetylic acid
319 Chalkone
1703 "Champignal"
347 Chavibetol
1866 *iso*-Chavibetol methyl ether
604 .... Chavicinic acid
605 .... *iso*-Chavicinic acid
606 .... Chavicol
2650 *iso*-Chavicol
90 Chavicol ethylether
1131 Chavicol methylether
2782 Chelidonic acid
2273 "Chinese seasoning"

*) see also summary of "Celery materials" included in this work at the end of the monographs in volume II, immediately preceding the index.

2791 Chinoleine
1186 Chloroacetic ester
607 .... *para*-Chloro benzyl acetate
614 *4*-Chloro-*3*,*5*-dimethylphenol
608 .... *2*-Chloro-*4*,*6*-dinitro-*1*,*3*-dimethyl-*5*-*tertiary*-butyl benzene
611 *para*-Chloro ethoxybenzene
611 *para*-Chloro ethyl phenol
609 .... Chloroform
2835 Chlorogalum pomeridianum
610 .... *meta*-Chloro hydrocinnamic aldehyde
614 *4*-Chloro-*5*-oxy-*1*,*3*-dimethylbenzol
613 *6*-Chloro-*3*-oxy-*1*-methyl-*4*-*iso*-propylbenzene
611 .... *para*-Chloro phenethole
610 *3*-Chloro phenylpropionic aldehyde
612 *omega*-Chlorostyrene
612 .... *omega*-Chlorostyrol
613 .... Chloro thymol
614 .... Chloro xylenol
614 *para*-Chloro-*meta*-xylenol
614 2-Chloro-*meta*-*5*-xylenol
1187 Chrysanthemic acid, ethylester
1187 Chrysanthemum-monocarboxylic acid, ethylester
2995 Chrystanthenone
2609 Chrystanthone
2235 Cincholepidine
1074 Cinene (see also 1800)
615 .... *1*,*4*-Cineole
616 .... *1*,*8*-Cineole
619 Cinnamal
619 *trans*-Cinnamaldehyde
620 Cinnamal diethyl acetal
622 Cinnamal dimethyl acetal
640 Cinnamal pulegone
641 "Cinnamalva"
299 "Cinnamein"
617 .... Cinnamic acid
618 .... Cinnamic alcohol
2496 "*iso*-Cinnamic alcohol"
619 .... Cinnamic aldehyde
620 .... Cinnamic aldehyde diethyl acetal
621 .... Cinnamic aldehyde-*2*,*4*-dihydroxy-*4*-methylpentane acetal
622 .... Cinnamic aldehyde dimethyl acetal
623 .... Cinnamic aldehyde ethylene glycol acetal
624 .... Cinnamic aldehyde-methylanthranilate
1372 Cinnamoyl eugenol
625 .... *1*-Cinnamoyl piperidine
626 .... Cinnamyl acetate
2495 "*iso*-Cinnamyl acetate"
618 Cinnamyl alcohol
627 Cinnamyl-*ortho*-aminobenzoate
627 .... Cinnamyl anthranilate
628 .... Cinnamyl benzoate
321 Cinnamyl-*iso*-butylidene ketone
629 .... Cinnamyl butyrate
630 .... Cinnamyl-*iso*-butyrate
631 .... Cinnamyl caproate
632 .... Cinnamyl caprylate
633 .... Cinnamyl cinnamate
646 Cinnamyl-*trans*-*alpha*-*beta*-dimethylacrylate
634 .... Cinnamyl ethoxyacetate
635 .... Cinnamyl eugenol
636 .... Cinnamyl formate
637 .... Cinnamyl heptoate
637 Cinnamyl heptylate
1529 Cinnamyl heptylether
631 Cinnamyl hexoate
645 Cinnamyl-*ortho*-hydroxybenzoate
320 Cinnamylidene acetaldehyde
2609 Cinnamylidene acetone
638 .... Cinnamylidene acetophenone
639 .... Cinnamylidene methylcarbinol (see also 1691)
640 .... Cinnamylidene pulegone
646 Cinnamyl-*trans*-*alpha*-methylcrotonate
641 .... Cinnamyl nitrile
642 Cinnamyl nonanoate
632 Cinnamyl octoate
642 .... Cinnamyl pelargonate
647 Cinnamyl-*n*-pentanoate
643 .... Cinnamyl phenylacetate
644 .... Cinnamyl propionate
645 .... Cinnamyl salicylate
646 .... Cinnamyl tiglate
647 .... Cinnamyl valerate (see also 648)
648 .... Cinnamyl-*iso*-valerate
623 "Cinncloval"
649 .... Citral
650 .... *iso*-Citral
651 .... Citral diethyl acetal
652 .... Citral dimethyl acetal
653 .... Citral enol acetate
653 *iso*-Citral enol acetate
654 .... Citral-indole
655 .... Citral-methylanthranilate
1003 "Citralone"
656 .... Citral propyleneglycol acetal
1451 "Citralva"
931 "Citral W"
2852 "Citratin"
1800 Citrene
2162 "Citrial"
657 .... Citric acid (see also 2854)
51 Citridic acid
2990 "Citroflex No. 2"
2972 "Citroflex A-4"
658 .... Citronellal
2771 "Citronellal acetylated"
659 .... Citronellal cyclo monoglycol acetal
660 .... Citronellal diethyl acetal
661 .... Citronellal dimethyl acetal
662 .... Citronellal di-phenylethyl acetal
663 .... Citronellal enol acetate (see also 2771)
659 Citronellal ethyleneglycol (cyclic) acetal
1728 Citronellal hydrate
664 .... Citronellal-Indole
665 .... Citronellal-Methylanthranilate
666 .... Citronellic acid
667 .... Citronellidene cyclohexanone
668 .... *alpha*-Citronellidene cyclopentanone
900 Citronellidene diethylmalonate

669 .... Citronellol
670 .... *laevo*-Citronellol
669 *dl*-Citronellol
1737 "Citronellol hydrate"
688 Citronelloxy acetaldehyde
671 .... Citronellyl acetate
672 .... Citronellyl anthranilate
673 .... Citronellyl benzoate
679 Citronellyl-*2*-butenoate
674 .... Citronellyl butyrate
675 .... Citronellyl-*iso*-butyrate
676 .... *alpha*-*n*-Citronellyl-*gamma*-butyrolactone
677 .... Citronellyl caproate
678 .... Citronellyl cinnamate
679 .... Citronellyl crotonate
679 Citronellyl-*alpha*-crotonate
680 .... *alpha*-Citronellyl cyclopentanone
693 Citronellyl-*trans*-*alpha*-*beta*-dimethylacrylate
1193 Citronellyl ethoxalate
681 .... Citronellyl ethoxyacetate
682 .... Citronellyl ethyl acetal
1193 Citronellyl ethyloxalate
683 .... Citronellyl formate
677 Citronellyl hexoate
677 Citronellyl hexylate
684 .... Citronellyl methoxyacetate
685 .... Citronellyl methyl acetal
1960 Citronellyl methyl ether (see also 1961)
686 .... Citronellyl monochloro acetate
687 .... Citronellyl oxalate
688 .... Citronellyl oxyacetaldehyde
689 .... Citronellyl oxyacetaldehyde diethyl acetal
690 .... Citronellyl phenylacetate
691 .... Citronellyl propionate
692 .... Citronellyl-*iso*-propoxyacetate
693 .... Citronellyl tiglate
694 .... Citronellyl valerate
695 .... Citronellyl-*iso*-valerate
696 .... Citronellyl vinyl ether
2852 "Citrosidine"
2384 "Citroviol"
697 .... Citrylidene acetaldehyde
2762 Citrylidene acetone
698 .... Citrylidene allyl acetone
699 .... *alpha*-Citrylidene cyclopentanone
2764 Citrylidene methyl-*iso*-butyl ketone
2765 Citrylidene methyl ethyl ketone
2917 "Civettal, cryst."
700 .... Civettone
2836 Clary sage
2291 Clavel moena oil
701 .... Clovene
736 "Coal tar creosote"
1965 "Cocodescol"
2350 "Coconut aldehyde"
558 Coffeine
1321 "Cognac oil, artificial"
167 "Coniferan"
702 .... *para*-Coniferaldehyde
703 .... Coniferyl alcohol
2745 Coniine
2745 Conyrine
1803 "Coriandrol"
1464 Corn sugar
1831 "Corps praline"
2734 "Cortexal"
1987 "Corylone"
2781 Coumalin
704 *cis*-*ortho*-Coumaric acid, anhydride
704 .... Coumarin
13 Crataegon
2638 Cream of tartar
2638 Cremor tartari
705 .... Creosol
1873 Creosol ethylether
1689 Creosol methylether
706 .... Creosote
724 "Cresatin"
707 .... *meta*-Cresol
708 .... *para*-Cresol
709 .... *para*-Cresol amylether
709 *para*-Cresol-*iso*-amylether
710 .... *para*-Cresol benzylether
711 .... *para*-Cresol-*n*-butylether
712 .... *meta*-Cresol ethylether
732 *ortho*-Cresol ethylether
713 .... *para*-Cresol ethylether
714 .... *meta*-Cresol heptylether
714 *meta*-Cresol heptyloxide
715 .... *ortho*-Cresol hexylether
716 .... *para*-Cresol hexylether
715 *ortho*-Cresol-*n*-hexyloxide
716 *para*-Cresol-*n*-hexyloxide
717 .... *meta*-Cresol methylether
718 .... *ortho*-Cresol methylether
719 .... *para*-Cresol methylether
720 .... *meta*-Cresol phenylether
721 .... *ortho*-Cresol phenylether
722 .... *para*-Cresol phenylether
723 .... *para*-Cresol propylether
2929 *para*-Cresol-tetrahydro-*2*-pyranyl-ether
724 .... *meta*-Cresyl acetate
2955 *ortho*-Cresyl acetate
725 .... *para*-Cresyl acetate
2964 *para*-Cresyl anthranilate
726 .... *para*-Cresyl benzoate
727 .... *para*-Cresyl benzoyl acetate
711 "Cresyl butyl oxide"
728 .... *para*-Cresyl butyrate
729 .... *para*-Cresyl-*iso*-butyrate
730 .... *para*-Cresyl caprylate
731 .... *para*-Cresyl cinnamate
742 *para*-Cresyl-*trans*-*alpha*-*beta*-dimethylacrylate
2969 *para*-Cresyl dodecanoate
732 .... *ortho*-Cresyl ether
1099 *para*-Cresyl ether
733 .... *para*-Cresyl ethylcarbonate
734 .... *para*-Cresyl formate
735 .... *para*-Cresyl heptyl ketone
741 *para*-Cresyl-*ortho*-hydroxybenzoate
2963 *2*-(*ortho*-*meta*-*para*-Cresyl)-*5*-hydroxy-dioxan
2963 *2*-(*ortho*-*meta*-*para*-Cresyl)-*5*-hydroxymethyl-dioxolan

736 .... Cresylic acid
2969 *para*-Cresyl laurate
730 *para*-Cresyl octoate
730 *para*-Cresyl octylate
732 *ortho*-Cresyl oxide
1099 *para*-Cresyl oxide
737 .... *meta*-Cresyl phenylacetate
738 .... *ortho*-Cresyl phenylacetate
739 .... *para*-Cresyl phenylacetate
740 .... *para*-Cresyl phenylcaprylate
740 *para*-Cresyl phenyloctanoate
722 "Cresyl phenyl oxide"
1923 "*para*-Cresyl propionate"
741 .... *para*-Cresyl salivate
742 .... *para*-Cresyl tiglate
743 .... *para*-Cresyl valerate
744 .... *para*-Cresyl-*iso*-valerate
1857 *iso*-Croton aldehyde
745 .... Crotonaldehyde-2-methylpentane-(*2,4*-diol)-acetal
73 Crotonic acid, nitrile
747 Crotonyl benzoate
748 Crotonyl heptylate
746 "Crotonyl mustard oil"
749 Crotonyl phenylacetate
746 .... Crotonyl-*iso*-thiocyanate
747 .... Crotyl benzoate
748 .... Crotyl heptoate
749 .... Crotyl phenylacetate
2694 Cryptone
1492 Cryptopyrrole
2857 "Crystallose"
2341 "Cucumber alcohol"
2339 "Cucumber aldehyde"
753 Cumaldehyde
1194 "Cumaran"
318 Cumaranol
1867 *para*-Cumaric alcohol methylether
1868 *ortho*-Cumaric aldehyde methylether
1868 *para*-Cumaric aldehyde methylether
704 Cumarin
750 .... Cumene
751 .... *para*-Cumenyl acetic acid
2738 *4*-Cumenylbutanol-*1*
756 Cumic acid
752 Cumic alcohol
757 Cuminacetate
753 Cuminal
752 .... Cuminalcohol
753 .... Cuminaldehyde
754 .... Cuminaldehyde dimethyl acetal
755 .... Cuminaldehyde-methylanthranilate
2734 Cuminic acetaldehyde
757 Cuminic acetate
756 .... Cuminic acid
753 Cuminic aldehyde
752 Cuminol
757 .... Cuminyl acetate
752 Cuminyl alcohol
2668 Cuminyl butyraldehyde
2739 Cuminyl carbinol
750 "Cumol"
2734 Cumyl acetaldehyde
17 Cumyl methyl ketone
1411 C.W.S.-fumaric acid
279 Cyanbenzol
1728 "Cyclalia"
758 Cyclamal
2725 "*iso*-Cyclamal"
2221 "Cyclamal cycloacetal"
2221 Cyclamal ethyleneglycol acetal
2222 Cyclamal monomethylacetal
2223 "Cyclamal acetate"
2220 "Cyclamen alcohol"
2223 Cyclamen alcohol, acetate
2224 Cyclamen alcohol, *n*-butyrate
2225 Cyclamen alcohol, propionate
758 .... Cyclamen aldehyde
759 .... Cyclamen aldehyde-methylanthranilate
2224 "Cyclamen butyrate"
2225 "Cyclamen propionate"
775 "Cyclamic acid"
2049 "Cyclamon" (Cyclamone)
758 "Cyclaviol"
1728 "Cyclia"
1214 Cyclic ethylene glycol ester of brassylic acid
760 .... Cyclocitral
760 *alpha*-Cyclocitral
760 *beta*-Cyclocitral
761 .... *iso*-Cyclocitral
761 "*meta*"-*iso*-Cyclocitral
761 *symmetric*-*iso*-Cyclocitral
1783 Cyclocitralone (see also 2212)
947 Cyclocitronellidene acetone
762 .... *alpha*-Cyclocitrylidene acetaldehyde
763 .... *beta*-Cyclocitrylidene acetaldehyde
764 .... Cyclocitrylidene acetonitrile
2085 *alpha*-Cyclocitrylidene butanone
2089 *gamma*-Cyclocitrylidene butanone (see also 2090)
765 .... *alpha*-Cyclocitrylidene-*4*-methylbutan-*3*-one
766 .... *alpha*-Cyclocitrylidene-*1*-methylpentan-*4*-one
1109 "Cyclododecalactone"
1728 "Cyclodor"
1214 Cyclo-*1,13*-ethylenedioxy tridecan-*1,13*-dione
767 .... *alpha*-Cyclogeraniol
768 .... *beta*-Cyclogeraniol
769 .... Cyclogeranyl methyl ketone
933 Cycloheptadecanone
700 Cycloheptadecen-*9*-one-*1*
770 .... Cyclohexadecane epoxide
923 Cyclohexadecanolide
771 .... Cyclohexadecanone
106 Cyclohexadecen-*5*-olide
107 Cyclohexadecen-*6*-olide
105 Cyclohexadecen-*7*-olide
281 *1,2*-Cyclohexadiene dione
282 *1,4*-Cyclohexadiene dione
781 Cyclohexane acetate
772 .... Cyclohexane acetic acid
163 Cyclohexane acetic acid, amylester
1199 Cyclohexane acetic acid, ethylester
773 Cyclohexane aldehyde diethyl acetal
774 Cyclohexane aldehyde dimethyl acetal

1657 Cyclohexane butyric acid, hexylester
773 .... Cyclohexane carboxaldehyde diethyl acetal
774 .... Cyclohexane carboxaldehyde dimethyl acetal
1202 Cyclohexane ethylacetate
1203 Cyclohexane ethylbutyrate
795 "Cyclohexane methylacetate"
164 Cyclohexane propionic acid, amylester
1200 Cyclohexane propionic acid, ethylester
775 .... Cyclohexane sulfamic acid
776 .... Cyclohexanol
777 .... Cyclohexanone
278 Cyclohexatriene
773 Cyclohexene carboxaldehyde diethyl acetal
774 Cyclohexene carboxaldehyde dimethyl acetal
778 .... Cyclohexen-*2*-one(*1*)
779 .... *3*-Cyclohexenone-*1*
2896 *3*-(Cyclohex-*3*-en-*1*-yl)-propen-*2*-al-*1*
780 .... Cyclohexyl acetaldehyde
781 .... Cyclohexyl acetate
772 Cyclohexyl acetic acid
782 .... Cyclohexyl anthranilate
783 .... Cyclohexyl benzoate
784 .... Cyclohexyl butyrate
785 .... Cyclohexyl-*iso*-butyrate
786 .... Cyclohexyl caproate
796 Cyclohexyl carbinol
787 .... Cyclohexyl cinnamate
788 .... *2*-Cyclohexyl cyclohexanol
789 .... *2*-Cyclohexyl cyclohexanone
790 .... *4*-Cyclohexyl cyclohexanone
791 *2*-Cyclohexyl ethanol
791 .... Cyclohexyl ethylalcohol
1200 Cyclohexyl ethylpropionate
773 Cyclohexylformaldehyde diethyl acetal
774 Cyclohexylformaldehyde dimethyl acetal
792 .... Cyclohexyl formate
793 .... Cyclohexyl heptoate
793 Cyclohexyl heptylate
794 .... Cyclohexylidene acetaldehyde
806 Cyclohexyl mercaptoacetate
795 .... Cyclohexyl methylacetate
796 .... Cyclohexyl methylalcohol
797 .... Cyclohexyl methyl-*iso*-butyrate
798 .... Cyclohexyl methylcrotonate
36 Cyclohexyl methyl ketone
799 .... Cyclohexyl methylpropionate
801 Cyclohexyl nonanoate
801 Cyclohexyl nonylate
793 Cyclohexyl oenanthate
800 .... Cyclohexyl oxalate
801 .... Cyclohexyl pelargonate
802 .... Cyclohexyl phenylacetate
803 .... *2*-Cyclohexyl propanol
804 .... *3*-Cyclohexyl propanol
805 .... Cyclohexyl propionate
775 Cyclohexyl sulfamic acid
806 .... Cyclohexyl thioglycolate
807 .... Cyclohexyl valerate
808 .... Cyclohexyl-*iso*-valerate
809 .... *gamma*-Cyclo-homogeraniol
1728 "Cyclo hydronal"
2998 "Cyclonol"
3003 "Cyclonol acetate"
810 .... Cyclopentadecanol
811 .... Cyclopentadecanolide
812 .... Cyclopentadecanolone
813 .... Cyclopentadecanone
814 .... Cyclopentanone
1205 Cyclopent-*2*-ene acetic acid, ethylester
1991 Cyclopentenyl acetic acid, methylester
815 .... Cyclopentenyl acrolein
1205 Cyclopentenyl ethylacetate
815 *3*-(Cyclopenten-*1'*-yl)-propen-*2*-al-*1*
758 Cyclosal
1728 Cyclosia base
1987 "Cyclotene"
1988 "Cyclotene butyrate"
1990 "Cyclotene propionate"
816 .... Cyclotridecanone
1488 "Cyclozingerone" (so-called)
817 .... Cyclyl acetate
818 .... Cyclyl ethylcarbonate
560 "Cylan"
819 .... *para*-Cymene
2734 *para*-Cymene-*7*-carboxaldehyde
752 *para*-Cymen-*7*-ol
573 *2-para*-Cymenol
2944 *3-para*-Cymenol
819 "Cymol"
573 Cymophenol
2944 *alpha*-Cymophenol
2734 Cymyl acetaldehyde
2739 *beta-para*-Cymylethanol
2446 *para*-Cymyl ethyl methyl ketone
2741 *para*-Cymyl propanal
759 "Cyranthiol"

**D**

1835 Dacrydium biforme (oil)
471 "Dalpac" FG
2102 "Damascenine"
1072 "Daphnetin"
116 "Daramin"
471 "D.B.P.C."
820 .... Deca-*2,4*-dienal
821 .... *2,4*-decadienoic acid
822 .... Decadienol
823 .... Decahydro-*beta*-naphthaldehyde
830 Decahydronaphthalone
824 .... *trans*-Decahydro-*beta*-naphthol
825 .... Decahydro-*beta*-naphthylacetaldehyde
826 .... *trans*-Decahydro-*beta*-Naphthyl acetate
1206 Decahydro-*beta*-naphthylacetic acid, ethylester
1994 Decahydronaphthylacetic acid, methylester
827 .... Decahydro-*beta*-naphthyl formate
1648 Decalactone (see also 1649)
828 .... *gamma-n*-Decalactone

829 .... *delta*-Decalactone
1994 Decalin-*2*-carboxylic-*2*-acetic acid, methylester
824 Decalinol
826 Decalinyl acetate
827 *beta*-Decalinylformate
824 *trans-beta*-Decalol
830 .... *beta*-Decalone
825 Decalyl ethanal
838 Decamethylene carbonate
837 Decamethylene glycol
838 *monomer*-Decamethyleneglycol carbonate
832 Decamethyleneglycol ethanedioic (cyclic) ester
831 Decamethyleneglycol propanedioic (cyclic) ester
831 .... Decamethylene malonate
832 .... Decamethylene oxalate
833 .... *n*-Decanal
834 .... Decanal diethyl acetal
835 .... Decanal dimethyl acetal
836 .... Decanal-methylanthranilate
3051 Decane-*alpha*-carboxylic acid
2837 Decane dioic acid
837 .... Decane diol
838 .... *1,10*-Decanediol carbonate
2346 Decanediol diacetate
2346 Decanediol monoacetate
839 .... Decane nitrile
840 .... Decanoic acid
1263 *iso*-Decanoic acid
833 *n*-Decanoic aldehyde
841 .... Decanol-*1*
828 Decanolide-*1,4*
829 Decanolide-*1,5*
2127 "*iso*-Decanolide"
2146 *2*-Decanone
848 Decanyl acetate
852 Decanyl-*iso*-butanoate
851 Decanyl butyrate
852 Decanyl-*iso*-butyrate
868 Decave
842 .... Decen-*2*-al
842 Decenaldehyde
843 .... *2*-Decenoic acid
843 *9*-Decenoic acid
843 *cis-4*-Decenoic acid
567 *iso*-Decenoic acid, vanillylamide
844 .... *omega*-Decenol
844 *9*-Decenol-*1*
845 *gamma-3*-Decenolactone
845 .... *7*-Decenolactone
1546 *3*-Decen-*2*-one
846 .... Decenyl acetate
846 *9*-Decen-*1*-yl acetate
847 .... Decenyl propionate
847 *9*-Decen-*1*-yl propionate
848 .... Decyl acetate
849 .... *iso*-Decyl acetate
2987 *n*-Decylacrolein
841 *3*-Decylalcohol
833 *n*-Decylaldehyde
1031 "*iso*-Decyl aldehyde" (see also 2047 and 2136)
834 *n*-Decylaldehyde diethyl acetal
835 *n*-Decylaldehyde dimethyl acetal
2989 *3*-Decyl allylalcohol
850 .... Decyl benzoate
857 Decyl-*2*-butenoate
851 .... Decyl butyrate
852 .... Decyl-*iso*-butyrate
853 .... *alpha-n*-Decyl-*gamma*-butyrolactone
854 .... *gamma-n*-Decyl-*gamma*-butyrolactone
3031 Decylcarbinol
856 Decylcinnamal
855 .... Decyl cinnamate
856 .... *alpha-n*-Decyl cinnamic aldehyde
857 .... Decyl crotonate
857 Decyl-*alpha*-crotonate
857 Decyl-*trans*-crotonate
839 Decyl cyanide
843 *2*-Decylenic acid
844 Decylenic alcohol
842 Decylenic aldehyde
858 .... Decyl ether
1209 Decyl ethyl ether
859 .... Decyl formate
1536 Decyl heptyl ether
861 Decyl hexadecanoate
840 Decylic acid
841 Decylic alcohol
836 "Decylique"
866 Decyl mercaptoacetate
859 Decyl methanoate
867 Decyl-*beta*-methyl butanoate
867 Decyl-*beta*-methyl butyrate
1998 Decyl methyl ketone
862 Decyl nonanoate
862 Decyl-*n*-nonylate
860 .... Decyl oxyacetaldehyde
861 .... Decyl palmitate
862 .... Decyl pelargonate
863 .... Decyl phenylacetate
2989 *3*-Decyl-*2*-propen-*1*-ol
864 .... Decyl propionate
865 Decyl pyroracemate
865 .... Decyl pyruvate
866 .... Decyl thioglycolate
867 .... Decyl-*iso*-valerate
3048 Decyl valerolactone
868 .... Decyl vinyl ether
2 Dehydro abietylalcohol
44 Dehydro acetic acid
2206 Dehydrocarvacrol methylether
2213 "Dehydro cyclamenaldehyde"
869 .... Dehydro-*beta*-cyclocitral
2207 Dehydro-*para*-cymene
870 .... Dehydro linalool
3057 Delphinic acid
2726 "Deltyl extra"
2729 "Deltyl prime"
913 D.E.P.
1464 "Dextropur"
1464 Dextrose
44 D.H.A.
871 .... Diacetin
872 .... Diacetyl
22 *alpha-beta*-Diacetylethane

873 Diacetyl glycerin
873 .... Diacetyl glycerol
2795 *1,3*-Diacetylresorcin
1576 Diallyl
82 Diallyl-*trans*-butenedioate
874 .... Diallyl disulfide
875 .... Diallyl ether
82 Diallyl fumarate
973 Diallyl glycol
876 .... Diallyl sulfide
5 Di-*iso*-amyl acetal
169 Di-*iso*-amyl ether
877 .... Diamylketone
877 Di-*n-amyl* ketone
189 Di-*iso*-amyl ketone
193 Diamyl malonate
193 Diamyl methane carboxylate
1394 Di-*iso*-amyl methylal
203 Diamyl oxalate
212 Di-*n*-amyl phthalate
221 Di-*iso*-amyl succinate
222 Di-*iso*-amyl tartrate
3054 Diamyl valeral
2346 Diasmol
2346 Diasmyl acetate
2775 *para*-Diazine
878 .... Dibenzofuran
1079 Dibenzyl
307 Dibenzyl disulfide
879 .... Dibenzylether
880 .... Dibenzyl ketone
2470 *2,4*-Dibenzyl-*5*-phenyl-*6*-hydroxy-*1,3*-dioxan
341 Dibenzyl succinate
881 .... *3,5*-Di-*tertiary*-butyl acetophenone
486 Di-*n*-butyl-*cis*-butene dioate
885 Di-*n*-butyl-*trans*-butene dioate
882 .... *4,4*-Dibutyl-*gamma*-butyrolactone
2363 Di-*iso*-butyl carbinyl acetate
883 .... Dibutyl catechol ketal
884 .... Di-*iso*-butyl catechol ketal
471 *2,6*-Di-*tertiary*-butyl-*para*-cresol
531 Di-*tertiary*-butyl decandioate
889 Di-*n*-butyl decane dioate
1395 Di butyl formal
885 .... Dibutyl fumarate
882 *4,4*-Dibutyl-*4*-hydroxybutyric acid, *gamma*-lactone
886 .... Dibutyl ketone
480 Di-*iso*-butyl ketone
486 Di-*n*-butyl maleate
487 Di-*n*-butyl malonate
487 Di-*n*-butyl methanedicarboxylate
887 .... *2,4*-Di-*tertiary*-butyl-*5*-methoxy benzaldehyde
887 *2,4*-Di-*tertiary*-butyl-*6*-methoxy benzaldehyde
888 *2,6*-Di-*iso*-butyl-*4*-methylpyridine
501 Di-*n*-butyl oxalate
516 Di-*iso*-butyl phthalate
888 .... Di-*iso*-butyl-*gamma*-picoline
487 Di-*n*-butyl propandioate
889 .... Dibutyl sebacate
533 Di-*n*-butyl succinate
890 .... Dibutyl sulfide
534 Di-*n*-butyl tartrate
486 Di-*n*-butyl toxilate
891 .... Di-*n*-butyryl
892 .... Di-*iso*-butyryl
2974 Dicalcium phosphate
893 .... Dichlorophenyl nitroethylene
894 .... Dicrotyl sulfide
895 .... Dicyclohexyl
896 .... Dicyclohexyl formal
896 Dicyclohexyl methylal
800 Dicyclohexyl oxalate
897 .... Dicyclopentadiene aldehyde
154 *1,1*-Diethoxy-*2*-amyl-*3*-phenyl-*2*-propene
588 *ortho*-Diethoxy benzene
1718 *para*-Diethoxy benzene
773 Diethoxy cyclohexylmethane
834 *1,1*-Diethoxy decane
6 *1,1*-Diethoxy ethane
2344 *9,9*-Diethoxy nonane
2398 *1,1*-Diethoxy octane
6 Diethyl acetal
1177 Diethyl acetaldehyde
1180 Diethyl acetic acid
2525 Diethylacetic acid, phenylethylester
19 Diethyl acetone
898 .... *omega-omega*-Diethyl acetophenone
1141 Diethyl aconitate
1143 Diethyl adipate
1155 Diethyl aminosuccinate
1230 “Diethyl anthranilate”
1155 *d*-Diethyl aspartate
899 .... Diethyl benzyl carbinol
588 “Diethyl catechol”
900 .... Diethylcitronellidene malonate
901 .... Diethyl citronellol
902 .... Diethyl diethylmalonate
1070 *1,4*-Diethylene dioxide
903 .... Diethyleneglycol dimethylether
904 .... Diethyleneglycol monoethylether
905 .... Diethyleneglycol monomethylether
2898 Diethylene oxide
912 Diethyl ethanedioate
906 .... Diethyl ether
1169 Diethyl ethylacetate
1649 *alpha*-(Diethyl-ethyl)-*gamma*-butyrolactone
1396 Diethyl formal
901 Diethyl geraniol
907 .... Diethyl glutamate
1143 Diethyl hexanedioate
908 Diethyl hydroxysuccinate
908 .... Diethyl malate
909 .... Diethyl maleate
910 .... Diethyl malonate
2653 Diethyl ketone
902 “Diethyl malonic ester”
1396 Diethyl methylal
911 .... Diethyl methylmalonate
912 .... Diethyl oxalate
913 .... Diethyl phthalate
914 .... Diethyl sebacate
915 .... Diethyl succinate
916 .... Diethyl tartrate
917 .... *2,5*-Diethyl tetrahydrofuran

918 .... Di-furfuryl disulfide
2383 "Diheptol"
2384 "Diheptyl acetate"
919 .... Diheptyl ether
920 .... Di-*beta*-*gamma*-Hexenylether
921 .... Dihexyl fumarate
922 .... Dihexyl ketone
923 .... Dihydro ambrettolide
924 .... Dihydro anethole
925 .... Dihydro-*n*-butylidene phthalide
926 .... Dihydro carveol
927 .... *cis*-Dihydro carvone
928 .... Dihydro carvylacetate
929 .... Dihydro carvyl benzoate
930 .... Dihydro citral
931 .... Dihydrocitronellal
932 .... Dihydrocitronellal dimethyl acetal
1032 Dihydrocitronellol
1033 Dihydrocitronellyl acetate
1034 Dihydrocitronellyl phenylacetate
933 .... Dihydrocivettone
934 .... Dihydrocoumarin
2692 Dihydrocryptol
2693 Dihydrocryptol acetate
937 Dihydro cuminic aldehyde
935 .... Dihydro cuminyl acetate
936 .... Dihydro cuminyl alcohol
937 .... Dihydro cuminyl aldehyde
938 .... Dihydro cuminyl aldehyde-*anti*-aldoxim
939 .... Dihydro cyclocitral
940 .... Dihydro cyclogeraniol
941 .... Dihydro cyclogeranyl acetate
942 .... Dihydro cyclol
1583 Dihydro cyclopentadiene aldehyde diethyl acetal
1584 Dihydro cyclopentadiene methanol acetate
1585 Dihydro cyclopentadiene oxyacetaldehyde
943 .... Dihydro cyclyl acetate
2619 "Dihydro-*para*-cymene"
2305 *1,4*-Dihydro-*1,4*-diketo-naphthalene
1886 "Dihydro ethone"
1272 Dihydro ethyl benzoyl acetate
944 .... Dihydro eugenol
2000 Dihydro eugenol methylether
945 Dihydro farnesene
945 .... Dihydro farnesol
946 .... Dihydro geraniol
2925 Dihydro geranyl acetate
947 .... *cis*-Dihydro ionone
948 .... Dihydro-*alpha*-ionone
949 .... Dihydro-*beta*-ionone
950 .... Dihydro-*gamma*-ionone
951 .... Dihydro-*alpha*-irone (and Dihydro-*iso*-*alpha*-irone)
952 .... Dihydro-*beta*-irone
953 .... Dihydro-*gamma*-irone
953 Dihydro-*iso*-*gamma*-irone
954 .... Dihydro jasmone (see also 1659)
955 .... Dihydro-*iso*-jasmone (see also 1659)
956 .... Dihydro jasmone lactone
2812 *1,2*-Dihydro-*2*-ketobenz-*iso*-sulfonazole
959 Dihydro-*iso*-lavandulal
957 .... *iso*-Dihydro lavandulol
958 .... *iso*-Dihydro lavandulyl acetate
957 *iso*-Dihydro lavandulyl alcohol
959 .... *iso*-Dihydro lavandulyl aldehyde
960 .... Dihydro linalool
1835 Dihydro manool
1570 Dihydro methylabietate
3009 Dihydro methylcamphene carbinol
2000 Dihydro methyleugenol
961 .... Dihydro-*alpha*-methyl ionone
962 .... Dihydro-*delta*-methyl ionone
962 Dihydro-*iso*-methyl-*beta*-ionone
963 .... Dihydro-*4*-(or -*3*)-(*4*-methyl-*3*-(or -*2*)-penten-*1*-yl)-*Δ3*-pyran
964 .... Dihydro myrcenol
965 .... Dihydro myrcenyl acetate
966 .... Dihydro-nor-Dicyclopentadienyl acetate
2520 Dihydro-*alpha*-phenylallyl alcohol
2998 Dihydro-*iso*-phorol
967 .... Dihydro-*iso*-phorone
1432 *alpha*-*beta*-Dihydro pseudoionone
1858 *2,3*-Dihydro-*gamma*-pyran-di-*alpha*-methallyl acetal
1858 *2,3*-Dihydro-*gamma*-pyran-di-methyl vinyl carbinyl acetal
968 .... Dihydro safrole
969 .... Dihydro-*alpha*-stilbazole
969 Dihydro-*2*-styryl pyridine
970 .... Dihydro-*alpha*-terpineol
971 .... Dihydro terpinyl acetate
2704 "Dihydrovanitrope"
972 .... Dihydroxy acetone
2761 *3,4*-Dihydroxy benzaldehyde
2793 *meta*-Dihydroxybenzene
1717 *para*-Dihydroxybenzene
448 *1,3*-Dihydroxybutane
2872 *L*-*2*,-*3*-Dihydroxybutane dioic acid
973 .... *3,4*-Dihydroxy-*1,5*-hexadiene
1071 *2,4*-Dihydroxy hexanal
1073 *3,4*-Dihydroxy-*5*-methoxy-*1*-*iso*-propylbenzene
2812 *2,3*-Dihydroxy-*3*-oxobenz-*iso*-sulfonazole
2696 *1,2*-Dihydroxy propane
972 *1,3*-Dihydroxypropan-*2*-one
2872 *dextro*-*alpha*-*beta*-Dihydroxy succinic acid
2796 *2,4*-Dihydroxy-*meta*-xylene
2796 *3,5*-Dihydroxy-*ortho*-xylene
1126 Di-hypnone
1774 Di-indolyl phenylethyl ethylene
974 .... Di-isoprene
872 *2,3*-Di-ketobutane
975 .... Dill apiole
976 .... Dill-*iso*-apiole
977 .... *2,5*-Dimethoxy acetophenone
978 .... *3,4*-Dimethoxy acetophenone
981 *3,5*-Dimethoxy-*4*-acetylphenol
2026 *1,2*-Dimethoxy-*4*-allylbenzene
979 .... *3,4*-Dimethoxy-*alpha*-amylcinnamic aldehyde

155 *1,1*-Dimethoxy-*2*-amyl-*3*-phenyl-*2*-propene
1057 *2,4*-Dimethoxy benzaldehyde
3077 *3,4*-Dimethoxy benzaldehyde
2796 *meta*-Dimethoxybenzene
3078 *ortho*-Dimethoxybenzene
3077 *3,4*-Dimethoxy benzenecarbonal
982 *3,4*-Dimethoxy benzylacetone
527 *1,3*-Dimethoxy-*4*-*tertiary*-butylbenzene
468 *1,4*-Dimethoxy-*2*-*tertiary*-butylbenzene
980 .... *3,4*-Dimethoxy cinnamic aldehyde
774 Dimethoxy cyclohexylmethane
2943 *2,5*-Dimethoxy-*para*-cymene
835 *10,10*-Dimethoxy decane
1731 *1,1*-Dimethoxy-*3,7*-dimethyloctan-*7*-ol
1106 *12,12*-Dimethoxy dodecane
1742 *3,5*-Dimethoxy-*4*-hydroxybenzaldehyde
2778 *1,3*-Dimethoxy-*2*-hydroxybenzene
1397 Dimethoxymethane
1689 *3,4*-Dimethoxy-*1*-methylbenzene
2345 *9,9*-Dimethoxy nonane
2399 *1,1*-Dimethoxy octane
981 .... *2,6*-Dimethoxy-*4*-oxyacetophenone
2778 *2,6*-Dimethoxy phenol
2069 *3,4*-Dimethoxy phenylacetaldehyde
982 *1(3,4*-Dimethoxyphenyl)-*3*-butanone
2485 *1,1*-Dimethoxy-*2*-phenylethane
982 .... *3,4*-Dimethoxy phenylethyl methyl ketone
1700 *1,1*-Dimethoxy-*2*-phenylpropane
2027 *1,2*-Dimethoxy-*4*-propenylbenzene
2000 *3,4*-Dimethoxy propylbenzene
236 *4:4*-Dimethoxy stilbene
2953 *2,5*-Dimethoxytoluene
1689 *3,4*-Dimethoxytoluene
2441 *3,5*-Dimethoxytoluene
3030 *omega*-*omega*-Dimethoxy undecane
2227 *asymmetric-Dimethylacetone*
2653 *symmetric*-Dimethylacetone
983 .... *2,4*-Dimethyl acetophenone
984 .... Dimethyl acrolein
238 *cis*-*2,3*-Dimethyl acrylic acid
2949 *trans*-*alpha*-*beta*-Dimethyl acrylic acid
2950 *trans*-Dimethyl acrylic aldehyde
20 Dimethylal acetone
985 .... *beta*-*beta*-Dimethyl allylalcohol
986 .... *5,5*-Dimethyl-*2*-*n*-amyl-*1,3*-dioxane
1890 *alpha*-*alpha*-Dimethyl anisalacetone
2106 "Dimethylanthranilate"
2002 *N,N*-Dimethylanthranilic acid, methylester
3099 *2,3*-Dimethylbenzaldehyde
987 .... *2,4*-Dimethyl benzaldehyde (see also 3099)
3099 *2,5*-Dimethylbenzaldehyde
3099 *2,6*-Dimethylbenzaldehyde
3099 *3,4*-Dimethylbenzaldehyde
3099 *3,5*-Dimethylbenzaldehyde
3096 Dimethylbenzene
988 .... *2,4*-Dimethyl benzyl acetate
2247 *para*-*alpha*-Dimethyl benzylalcohol
1042 *alpha*-*alpha*-Dimethyl benzyl-*iso*-butyrate
989 .... Dimethyl benzyl carbinol
990 .... *iso*-Dimethyl benzyl carbinol
991 .... Dimethyl benzyl carbinyl acetate
992 .... Dimethyl benzyl carbinyl butyrate
993 .... Dimethyl benzyl carbinyl-*iso*-butyrate
994 .... Dimethyl benzyl carbinyl formate
995 .... Dimethyl benzyl carbinyl propionate
2471 *4,5*-Dimethyl-*2*-benzyl-*1,3*-dioxolan
2833 *2,3*-Dimethylbicyclo-(*1,2,2*)-heptene-*2*
2383 *6,6*-Dimethylbicyclo-(*3,1,1*)-*2*-heptene-*2*-ethanol
2384 *6,6*-Dimethylbicyclo-(*3,1,1*)-*2*-heptene-*2*-ethylacetate
996 .... *2,4*-Dimethyl butadiene acrolein
2616 *2,3*-Dimethyl-*2,3*-butanediol
2617 *2,3*-Dimethyl-*2,3*-butanediol dimethylether
2618 *2,2*-Dimethylbutan-*3*-one
2618 *3,3*-Dimethylbutan-*2*-one
1187 *1,1*-Dimethyl-*3*-*iso*-butenyl-cyclopropanoic acid, ethylester
997 .... *3,4*-Dimethyl-*7*-*tertiary*-butyl coumarin
980 Dimethyl caffeic aldehyde
1943 Dimethyl-*trans*-campholate
2661 Dimethyl carbinol
2658 Dimethyl carbinyl acetate
903 Dimethyl carbitol
998 .... Dimethyl carbonate
999 .... Dimethyl citronellol
2015 *2,4*-Dimethyl crotonaldehyde
2672 Dimethyl cuminyl carbinol
996 *2,4*-Dimethyl-*3*-cyclohexene aldehyde
996 *4,6*-Dimethyl-*3*-cyclohexene aldehyde
1061 *3,4*-Dimethyl cyclohex-*5*-enyl carboxaldehyde
1062 *alpha*-*alpha*-Dimethyl-*beta*-cyclohexen-*3*-yl ethanol
1000 .... *1,1*-Dimethyl cyclohex-*3*-enyl methyl ketone
1001 .... *1*-(*2,3*-Dimethylcyclohexyl)-*1*-buten-*3*-one
1002 .... *1*-(*3,5*-Dimethylcyclohexyl)-*1*-buten-*3*-one
1743 *alpha*-*alpha*-Dimethyl cyclohexylethyl methylcarbinol
1003 .... *5,9*-Dimethyl-*4,8*-decadien-*2*-one
1058 Dimethyldecane dioate
697 *2,6*-Dimethyl-*2,6,8*-decatrien-*10*-al
1004 .... *5,9*-Dimethyl-*8*-decen-*3*-ol
1055 *2,5*-Dimethyl-*1,4*-diazine
1056 *2,6*-Dimethyl-*1,4*-diazine
394 *2,2*-Dimethyl-*4,4*-dimethylhexan-*3*-one
1187 *1,1*-Dimethyl-*3*-(*beta*-*beta*-dimethylvinyl)-cyclopropanoic acid, ethylester
2279 *2,6*-Dimethyl-*3,5*-dinitro-*4*-*tertiary*-butylacetophenone

1468 *2,2*-Dimethyl-*1,3*-dioxolane-*4*-methanol
1089 *2,4*-Dimethyl-*3,5*-di-*iso*-propylbenzaldehyde
1005 .... *1,1*-Dimethyl-*5,7*-di-*iso*-propyl-*6*-indanol
1006 .... Dimethyl disulfide
1248 *6,10*-Dimethyl dodecadien-*5,9*-one-*2*
1007 .... *10,11*-Dimethyl dodecanal
2765 *2,6*-Dimethyldodeca-*2,6,8*-trien-*10*-one
1007 *alpha-beta*-Dimethyl dodecylaldehyde
60 *1,6*-Dimethyl-*2,3*- and *5,7*-*bis*-epoxy-*4*-octene
2154 Dimethyl ethanedioate
1008 .... Dimethyl ethyl carbinol
121 Dimethyl ethyl carbinyl acetate
1931 *2,6*-Dimethyl-*4*-ethyl-*4*-heptanol
1211 *2,2*-Dimethyl-*3*-(ethylphenyl)-propanal-*1*
2031 "Dimethylfuranaldehyde"
1742 "Dimethyl gallic aldehyde"
872 Dimethyl glyoxal
1009 .... *2,6*-Dimethyl heptadiene-(*1,5*)
1009 *2,6*-Dimethyl-*2,6*-heptadiene
1010 .... *4,6*-Dimethyl heptadien-(*3,5*)-ol-(*1*)
1011 *2,6*-Dimethyl heptaldehyde
480 *2,6*-Dimethylheptan-*4*-one
1011 .... *2,6*-Dimethyl-*2*-heptenal-(*7*)
1012 .... Dimethyl heptenol
1012 *2,6*-Dimethyl-*5*-heptenol
1012 *2,6*-Dimethyl-*2*-hepten-*6*-ol
1013 .... Dimethyl heptenyl acetate
1014 .... Dimethyl heptenyl-*iso*-butyrate
1015 .... Dimethyl heptenyl formate
1016 .... Dimethyl heptenyl propionate
1743 *alpha-alpha*-Dimethyl hexahydrophenylethyl methyl carbinol
1017 .... Dimethyl hexanediol
1942 *3,5*-Dimethyl-*2,4*-hexanedione
1018 .... *2,4*-Dimethylhexen-*4*-al-*6*
393 *6,6*-Dimethyl-*1*-hexen-*4*-ol
1019 .... *2,2*-Dimethyl-*4*-*iso*-hexyl cyclohexanone
1020 .... *2,4*-Dimethyl-*6*-*iso*-hexyl cyclohexanone
1021 .... *2,6*-Dimethyl-*4*-*iso*-hexyl cyclohexanone
1022 .... *3,4*-Dimethyl-*6*-*iso*-hexyl cyclohexanone
1023 .... *3,5*-Dimethyl-*2*-*iso*-hexyl cyclohexanone
2197 Dimethyl hydrocinnamyl carbinol
2583 "Dimethyl hydrocinnamyle"
1719 "Dimethyl hydroquinone"
1024 .... *alpha-beta*-Dimethyl-*gamma*-hydroxy-*gamma-n*-butyl-*2*-butenolide
809 *1,1*-Dimethyl-*2* (*beta*-hydroxyethyl)-*3*-methylene cyclohexane
1025 .... *2,5*-Dimethyl-*4*-hydroxy-*3*-(*2H*)-furanone
1468 *2,2*-Dimethyl-*4*-hydroxymethyl-*1,3*-dioxolane
1794 *2,6*-Dimethyl-*5*-hydroxymethyl heptadiene-*2,6*
2909 *2,6*-Dimethyl-*5*-hydroxymethyl heptane
957 *2,6*-Dimethyl-*2*-hydroxymethyl-*2*-heptene
957 *2,7*-Dimethyl-*6*-hydroxy-*4*-octene
990 *alpha-alpha*-Dimethyl-*beta*-hydroxyphenyl ethylene
1479 *1,4*-Dimethyl-*7*-(*alpha*-hydroxy-*iso*-propyl)-*Δ9,10*-octahydroazulene
1480 *1,4*-Dimethyl-*7*-(*alpha*-hydroxy-*iso*-propyl)-*Δ9,10*-octahydroazulene acetate
1026 .... Dimethyl indole
1026 *alpha-beta*-Dimethyl indole
1026 *1,3*-Dimethyl indole
1026 *2,3*-Dimethyl indole
1026 *2,5*-Dimethyl indole
1026 *3,4*-Dimethyl indole
765 Dimethyl ionone
765 *1,3*-Dimethyl-*alpha*-ionone
43 Dimethyl ketol
18 "Dimethyl ketone" (see also 872)
1024 *2,3*-Dimethyl-*4*-keto-*2*-nonenoic acid, enol-lactone
2098 Dimethyl malonate
1870 *3,7*-Dimethyl-*7*-methoxy-*1*-octanal
970 Dimethyl-(*4*-methylcyclohexyl)-carbinol
809 *2*-(*6,6*-Dimethyl-*2*-methylene)-cyclohexyl ethanol
1027 .... *2,6*-Dimethyl-*10*-methylene dodeca-*2,6,11*-trien-*1*-al
562 *2,2*-Dimethyl-*3*-methylene norbornane
562 *3,3*-Dimethyl-*2*-methylene norbornane
2847 *2,6*-Dimethyl-*8,8*-*bis*-(*3*-methyl-*3H*-indol-*3*-*yl*)-*2*-octanol
2005 Dimethyl methylpropane dioate
1187 *2,2*-Dimethyl-*3*-(*2*-methylpropenyl)-cyclopropanecarboxylic acid, ethyl ester
1478 *2,3*-Dimethyl naphthalene
1190 *3,7*-Dimethyl-*2,6*-nonadien-*1*-al
1279 *3,7*-Dimethyl-*1,6*-nonadien-*3*-ol
1246 *2*-*trans*-*3,7*-Dimethyl-*2,6*-nonadien-*1*-ol
1280 *3,7*-Dimethyl-*1,6*-nonadien-*3*-yl acetate
189 *2,8*-Dimethylnonan-*5*-one
1192 *3,7*-Dimethyl-*6*-nonen-*1*-ol
460 *6,8*-Dimethyl-*5*-nonen-*2*-one
1007 "Dimethyl nonyl acetaldehyde"
1028 .... *3,3*-Dimethyl-*Δ2*, *beta*-norbornane-*2*-ethanol
1029 .... *3,3*-Dimethyl-*Δ2*, *beta*-norbornane-*2*-ethylacetate
650 *3,7*-Dimethyl-*3,6*-octadienal
651 *3,7*-Dimethyl-*2,6*-octadienal diethyl acetal
652 *3,7*-Dimethyl-*2,6*-octadienal dimethyl acetal
974 *2,6*-Dimethyl-*2,6*-octadiene

974 *2,7*-Dimethyl-*2,6*-octadiene
974 *3,6*-Dimethyl-*2,6*-octadiene
1451 *3,7*-Dimethyl-*2,6*-octadiene-*1*-nitrile
1425 *3,7*-Dimethyl-*2,6* (and *2,7*)-octadienoic acid
2389 *2,6*-Dimethyl-*3,5*-octadien-*2*-ol
2389 *2,6*-Dimethyl-*5,7*-octadien-*2*-ol
1030 .... *2,7*-Dimethyl-*1,6*-octadien-*3*-ol (see also 1803)
1427 *3,7*-Dimethyl-*3,6*-octadienol
2315 *2-cis-3,7*-Dimethyl-*2,6*-octadien-*1*-ol
1426 *2-trans-3,7*-Dimethyl-*2,6*-octadien-*8*-ol
2390 *cis-2,6*-Dimethyl-*5,7*-octadien-*2*-yl acetate
1430 *trans-2,6*-Dimethyl-*2,6*-octadien-*8*-yl acetate
1806 *3,7*-Dimethyl-*1,6*-octadien-*3-yl* acetate
2322 *2-cis-3,7*-Dimethyl-*2,6*-octadien-*1*-yl acetate
1822 *3,7*-Dimethyl-*1,6*-octadien-*3*-yl acetylformate
1459 *trans-3,7*-Dimethyl-*2,6*-octadien-*8*-yl-*trans-alpha-beta*-acrylate
1436 *trans-3,7*-Dimethyl-*2,6*-octadien-*8*-yl-*n*-butyrate
1437 *trans-3,7*-Dimethyl-*2,6*-octadien-*8*-yl-*iso*-butyrate
1815 *3,7*-Dimethyl-*1,6*-octadien-*3*-yl formate
1446 *trans-3,7*-Dimethyl-*2,6*-octadienyl formate
1440 *trans-3,7*-Dimethyl-*2,6*-octadienyl hexanoate
1458 *trans-3,7*-Dimethyl-*2,6*-octadienyl-*ortho*-hydroxybenzoate
1453 *trans-3,7*-Dimethyl-*2,6*-octadienyl nonanoate
1441 *trans-3,7*-Dimethyl-*2,6*-octadienyl octanoate
1460 *trans-3,7*-Dimethyl-*2,6*-octadienyl pentanoate
1461 *trans-3,7*-Dimethyl-*2,6*-octadienyl-*iso*-pentanoate
1454 *trans-3,7*-Dimethyl-*2,6*-octadienyl phenylacetate
1442 *trans-3,7*-Dimethyl-*2,6*-octadienyl-*beta*-phenylacrylate
1821 *3,7*-Dimethyl-*1,6*-octadien-*3*-yl propanoate
1456 *trans-3,7*-Dimethyl-*3,6*-octadienyl propionate
1031 .... *3,6*-Dimethyl octanal
931 *3,7*-Dimethyl octanal
932 *3,7*-Dimethyl octanal dimethyl acetal
1737 *3,7*-Dimethyloctan-*1,7*-diol
1031 *2,6*-Dimethyl octanoic aldehyde
1032 .... Dimethyl octanol
2920 *2,6*-Dimethyl-*2*-octanol
1032 *2,6*-Dimethyloctan-*8*-ol
1032 *3,7*-Dimethyloctanol-*1*
2913 *3,7*-Dimethyl octanol-*3*
1033 .... Dimethyl octanyl acetate
849 *2,6*-Dimethyl octanyl acetate
2914 *3,7*-Dimethyl octan-*3-yl* acetate
1034 .... Dimethyl octanyl phenylacetate
59 *2,6*-Dimethyl-*1,5,7*-octatriene
2388 *3,7*-Dimethyl-*1,3,6*-octatriene
930 *3,7*-Dimethyl-*2*-octen-*1*-al
658 *3,7*-Dimethyl-*6*-octen-*1*-al
666 *3,7*-Dimethyl-*6*-octen-*6*-oic acid-*1*
1035 .... Dimethyl octenol
669 *3,7*-Dimethyl-*6*-octen-*1*-ol
960 *3,7*-Dimethyl-*6*-octen-*3*-ol
1035 *3,7*-Dimethyl-*7*-octen-*1*-ol
1036 .... Dimethyl octenyl acetate
671 *3,7*-Dimethyl-*6*-octen-*1*-yl acetate
1036 *3,7*-Dimethyl-*7*-octen-*1*-yl acetate
674 *3,7*-Dimethyl-*6*-octen-*1*-yl-*n*-butyrate
675 *3,7*-Dimethyl-*6*-octen-*1*-yl-*iso*-butyrate
693 *3,7*-Dimethyl-*6*-octen-*1*-yl-*trans-alpha*-methyl crotonate
694 *3,7*-Dimethyl-*6*-octen-*1*-yl pentanoate
695 *3,7*-Dimethyl-*6*-octen-*1*-yl-*iso*-pentanoate
690 *3,7*-Dimethyl-*6*-octen-*1*-yl phenylacetate
691 *3,7*-Dimethyl-*6*-octen-*1*-yl propionate
1794 *2,6*-Dimethylol-*5*-heptadiene-*2,6*
2154 Dimethyl oxalate
688 *6,10*-Dimethyl-*3*-oxa-*9*-undecenal
1174 *2,2*-Dimethylpentan-*3*-one
1037 .... *2,4*-Dimethyl phenylacetaldehyde
1038 .... *2,4*-Dimethyl phenylacetaldehyde diethyl acetal
1039 .... *ortho-para*-Dimethyl phenylallyl ether
1040 .... Dimethyl phenyl carbinol
1041 .... Dimethyl phenyl carbinyl acetate
1042 .... Dimethyl phenyl carbinyl-*iso*-butyrate
991 *alpha-alpha*-Dimethyl phenylethyl acetate
989 *alpha-alpha*-Dimethyl phenylethyl alcohol
992 *alpha-alpha*-Dimethyl phenylethyl-*n*-butyrate
993 *alpha-alpha*-Dimethyl phenylethyl-*iso*-butyrate
1043 .... Dimethyl phenylethyl carbinol
1044 .... Dimethyl phenylethyl carbinyl acetate
1045 .... Dimethyl phenylethyl carbinyl-*n*-butyrate
1046 .... Dimethyl phenylethyl carbinyl-*iso*-butyrate
1047 .... Dimethyl phenylethyl carbinyl formate
1048 .... Dimethyl phenylethyl carbinyl propionate
1049 .... Dimethyl phenylethyl carbinyl-*iso*-valerate
944 *alpha-alpha*-Dimethyl phenylethyl formate
2199 *alpha-alpha*-Dimethyl phenylethyl methylcarbinol
1050 .... *2,5*-Dimethyl-*5*-phenyl-*1*-hexen-*3*-one
1043 *1,1*-Dimethyl-*3*-phenylpropanol-*1*

2197 Dimethyl phenyl propyl carbinol
1051 .... Dimethyl phthalate
3053 *3,3*-Dimethyl propanal
2098 Dimethyl propane dioate
2156 *2,2*-Dimethyl-*1,3*-propanediol
2382 *5,6*-Dimethyl-*8*-*iso*-propenyl bicyclo (*4:4:0*)-dec-*1*-en-*2*-one
1478 *1,4*-Dimethyl-*7*-*iso*-propenyl-*Δ9,10*-octahydroazulene
2842 *1,10*-Dimethyl-*7*-*iso*-propenyl octahydronaphthalene
1174 *2,2*-Dimethyl propione
1053 *1,6*-Dimethyl-*4*-*iso*-propyl decalinol
1463 *1,7*-Dimethyl-*4*-*iso*-propylidene cyclodecadien-*6,10*-one
3089 *4,8*-Dimethyl-*2*-*iso*-propylidene-*6*-oxo-*cis*-*Δ4*-octahydroazulene
1052 *1,5*-Dimethyl-*3*-*iso*-propyl naphthalene
1052 .... *1,7*-Dimethyl-*4*-*iso*-propyl naphthalene
1053 .... *1,6*-Dimethyl-*4*-*iso*-propyl-oxy-decahydronaphthalene
1054 .... *2,4*-Dimethyl-*6*-*iso*-propylphenol
1055 .... *2,5*-Dimethyl pyrazine
1056 .... *2,6*-Dimethyl pyrazine
1827 *2,4*-Dimethyl pyridine
1826 *2,6*-Dimethyl pyridine
2796 "Dimethyl resorcinol"
2796 *2,4*-Dimethyl resorcinol
2796 *2,5*-Dimethyl resorcinol
2796 *4,5*-Dimethyl resorcinol
2796 *4,6*-Dimethyl resorcinol
1057 .... *para*-Dimethyl resorcylic aldehyde
1877 "Dimethyl salicylate"
1058 .... Dimethyl sebacate
1059 .... Dimethyl succinate
2005 Dimethyl-*iso*-succinate
1060 .... Dimethyl sulfide
996 *2,4*-Dimethyl tetrahydrobenzaldehyde
1061 .... *3,4*-Dimethyl-*Δ5*-tetrahydrobenzaldehyde
1062 .... Dimethyl tetrahydrophenylethyl alcohol
1063 .... Dimethyl tetrasulfide
2003 Dimethyl-*para*-tolylcarbinol
1064 .... *2,2*-Dimethyl-*3*-(*2,6,6*-trimethyl-*2*-cyclohexen-*1*-yl)-propionitrile
2254 Dimethyl trisulfide
1432 *2,6*-Dimethyl-undedadien-*2,6*-one-*10*
1588 *6,10*-Dimethyl-undecan-*2*-one
2762 *2,6*-Dimethyl-undeca-*2,6,8*-trien-*10*-one
2925 *6,10*-Dimethyl-*9*-undecen-*2*-one
1924 Dimethyl vinyl carbinol
1065 .... Dinitro-*tertiary*-butyl pseudo cumene
1066 .... Dinitro-*tertiary*-butyl xylene aldehyde
1067 .... Dinitro-*tertiary*-butyl xylyl cyanide
2279 *2,6*-Dinitro-*3,5*-dimethyl-*4*-acetyl-*tertiary*-butylbenzene
1066 Dinitro dimethyl butyl benzaldehyde
1067 *3,5*-Dinitro-*2,6*-dimethyl-*4*-*tertiary*-butyl benzonitrile
1068 .... *2,4*-Dinitro-*3*-ethyl-*6*-*tertiary*-butylanisole
2278 *2,6*-Dinitro-*3*-methoxy-*6*-*tertiary*-butyltoluene
2278 *2,6*-Dinitro-*3*-methoxy-*1*-methyl-*4*-*tertiary*-butylbenzene
2278 *2,4*-Dinitro-*3*-methyl-*6*-*tertiary*-butylanisole
2281 *2,6*-Dinitro-*3,4,5*-trimethyl-*tertiary*-butylbenzene
2429 Di-octyl malonate
2429 Di-*n*-octyl propane dioate
1411 Di-octyl sodium sulfosuccinate
182 "Di-oenanthal"
1069 .... Diosphenol
1070 .... Dioxane
1070 Dioxan-*1,4*
1402 *1,3*-Dioxolan
1402 *meta*-Dioxolane
1831 *3,4*-Dioxo-*2*-methyl-*2,3*-dihydro-*1,4*-pyran
1831 *3,4*-Dioxo-*2*-methyl-(*1,4*-pyran)-dihydride
2761 *3,4*-Dioxybenzaldehyde
1071 .... *alpha*-*gamma*-Dioxy-*n*-caproic aldehyde
1072 .... *7,8*-Dioxy coumarin
1073 .... *3,4*-Dioxy-*5*-methoxy-*iso*-propylbenzene
1484 Dioxymethylene protocatechuiuc aldehyde
45 *beta*-*gamma*-Dioxypentane
1074 .... Dipentene
2880 Dipentene glycol
1075 .... Dipentene tetrol
1076 .... Di-*beta*-pentenyl tetrasulfide
3054 Dipentoxy pentane
1077 .... Diphenyl
880 *alpha*-*alpha'*-Diphenyl acetone
2508 *trans*-*alpha*-*beta*-Diphenylacrylic acid
1078 .... Diphenylamine
1126 *1,3*-Diphenyl-*2*-buten-*1*-one
275 Diphenyl carbinol
878 Diphenylene oxide
1079 .... Diphenyl ethane
2007 *asymmetric*, *alpha*-*alpha*-Diphenyl ethane
1081 Diphenylether
2864 *trans*-*alpha*-*beta*-Diphenylethylene
2546 Diphenylethyl ethanedioate
280 Diphenyl ketone
1080 .... Diphenyl methane
1081 .... Diphenyl oxide
638 *1,5*-Diphenyl-*1,3*-pentadien-*5*-one
1082 .... Di-*5*-phenyl-*2*-(and-*3*-)-pentenoyl piperazone
289 *1,3*-Diphenylpropan-*1*-one
880 *1,3*-Diphenyl-*2*-propanone
319 *1,3*-Diphenyl-*2*-propen-*1*-one
1083 .... Di-*5*-phenyl-*n*-valeroyl piperazone
570 *iso*-Diprene
1084 .... Dipropionyl
9 Di-propyl acetal
1085 .... Di-*iso*-propyl acetophenone
1085 *3,5*-Di-*iso*-propyl-*1*-acetylbenzene
2659 Di-*iso*-propyl adipate
1086 .... Di-*iso*-propyl benzaldehyde

1087 .... Di-*iso*-propyl benzylacetate
2659 Di-*iso*-propyl-*1:4*-butane-dicarboxylate
2909 *2,4*-Di-*iso*-propyl-*1*-butanol
1088 .... Dipropyl carbinol
589 Di-*n*-propyl catechol ketal
590 Di-*iso*-propyl catechol ketal
2750 Di-*iso*-propyl decane dioate
891 Dipropyl diketone
892 Di-*iso*-propyl diketone
1089 .... Di-*iso*-propyl dimethyl benzaldehyde
2695 Di-*n*-propyl disulfide
2703 Di-*iso*-propyl ether
1398 Dipropyl formal
2659 Di-*iso*-propyl hexane dioate
1090 .... Dipropyl ketone
1091 .... Dipropyl malonate
1092 .... Di-*iso*-propyl methylbenzaldehyde
1093 .... Dipropyl oxalate
2703 Di-*iso*-propyloxide
1094 .... *2,4*-Di-*iso*-propyl phenylacetaldehyde
1095 .... Di-*iso*-propyl saligenin ketal
2750 Di-*iso*-propyl sebacate
1096 .... Dipropyl succinate
1092 *3,5*-Di-*iso*-propyl-*4*-tolylaldehyde
2753 Dipropyl trisulfide
52 Disacryl
1097 .... Disodium guanylate
1098 .... Disodium inosinate
1080 Ditane
568 Dithiocarbonic anhydride
1099 .... Ditolyl ether
1100 .... Di-*para*-tolyl methane
1412 Di-vinylene oxide
2783 Di-vinylenimine
3095 Di-vinylsulfide
989 D.M.B.C.
990 "*iso*-D.M.B.C." (see also 2021 and 2071)
991 D.M.B.C.A.
2022 "*iso*-D.M.B.C.A."
992 D.M.B.C. butyrate
995 D.M.B.C. propionate
1032 D.M.O.
1033 D.M.O. acetate
1034 D.M.O. phenylacetate
1051 D.M.P.
1040 D.M.P.C.
1041 D.M.P.C.A.
1043 D.M.P.E.C.
1044 D.M.P.E.C. acetate
1045 D.M.P.E.C. butyrate
1046 D.M.P.E.C.-*iso*-butyrate
1047 D.M.P.E.C. formate
1048 D.M.P.E.C. propionate
1049 D.M.P.E.C.-*iso*-valerate
1101 .... Dodeca-*2,4*-dien-*1*-al
1391 Dodecahydro-*3a,6,6,9a*-tetramethyl-(*2,1-b*)-furan
2414 *alpha*-Dodecalactone
1102 .... *gamma*-Dodecalactone
1103 .... *delta*-Dodecalactone
1104 .... Dodecamethylene carbonate
1105 .... Dodecanal
2132 "*iso*-Dodecanal"
1106 .... Dodecanal dimethyl acetal
2985 Dodecan-*1*-carboxylic acid
1120 *1*-Dodecanethiol
1107 .... Dodecanoic acid
1105 Dodecanoic aldehyde
1121 Dodecanoic nitrile
1108 .... Dodecanol
1102 Dodecanolide-*1:4* (see also 2414)
1109 .... *1,12*-Dodecanolide
2414 *alpha*-Dodecanolide
882 "Dodecanolide"
1998 Dodecan-*2*-one
1113 Dodecanyl acetate
1110 .... *n*-Dodecen-*2*-al
1110 *trans*-*2*-Dodecen-*1*-al
1111 .... Dodecenol
1112 .... Dodecenyl propionate
1107 Dodecoic acid
1113 .... *n*-Dodecyl acetate
1108 Dodecyl alcohol, ***n-primary***
1114 .... Dodecyl benzoate
1115 .... Dodecyl butyrate
1116 .... Dodecyl-*iso*-butyrate
1117 .... *alpha*-Dodecyl-*gamma*-butyrolactone
1118 .... Dodecyl cyclohexanol
1111 Dodecylenic alcohol
1119 .... Dodecyl formate
1537 Dodecyl heptylether
1105 Dodecylic aldehyde
1109 Dodecyllactone-*1:12*
1120 .... Dodecyl mercaptan
1121 .... Dodecyl nitrile
1122 .... Dodecyl propionate
1123 .... Dodecyl valerate
1124 .... Dodecyl-*iso*-valerate
2943 "Dog Fennel"
440 "Dorisyl"
245 "Draconic acid"
276 "Dracylic acid"
2346 "Drago-Jasimia"
1125 .... Dulcin
1488 "Dulcinyl"
814 Dumasin
2994 Durylic acid, nitrile
2994 Durylonitrile
1074 "Dycom"
1126 .... Dypnone

**E**

1148 E.A.K.
1696 Ecorsal (see also 2954)
2854 E.D.T.A.
404 "Eglantine" (see also 510)
2440 *trans*-Elaidic acid
2440 Elain
1127 .... Elemicine
423 "Eliminoxy"
1128 .... Elemol
1129 .... Elemyl acetate
1930 "Elsholtzia ketone"
1930 Elsholtzione
469 Embanox
1309 E.M.-*para*-M.P.G.
1306 E.M.P.G.

1494 Enanthal
1494 Enanthaldehyde
1513 Enanthic acetate
1500 Enanthic acid
1501 Enanthic alcohol
1501 Enanthyl alcohol
904 Enkanol
2971 "Enzactin"
13 Epenone
1339 E.P.G.
1804 "Epoxy dihydrolinalool"
1226 *1,2*-Epoxy ethane
1780 Epoxy-*2,3*-*beta*-ionone
1804 Epoxy linalool
1805 "Epoxy linalyl acetate"
615 *1,4*-Epoxy-*para*-menthane
616 *1,8*-Epoxy-*para*-menthane
1288 *alpha-beta*-Epoxy-*beta*-(*para*-methoxyphenyl)-propionate
2866 *1,2*-Epoxy-*1*-phenylethane
2562 *alpha-beta*-Epoxy-*beta*-phenylpropionic acid
51 Equisetic acid
1878 Ericin
1130 .... Erythorbic acid
1131 Esdragol
13 Estenone
1131 .... Estragole
236 *iso*-Estragole
1136 Ethacol
1574 Ethal
3 Ethanal
1215 Ethane diol
16 Ethanoic acid
1144 Ethanol
1132 .... *2*-Ethanol piperidine
1914 Ethenyl aminophenol
868 Ethenyl oxydecane
906 Ether
1133 .... Ethinyl cyclohexylacetate
1907 "Ethone"
1363 "Ethovan"
1134 .... *ortho*-Ethoxy acetophenone
1134 *1*-Ethoxy-*2*-acetylbenzene
90 *4*-Ethoxy-*1*-allylbenzene
1474 *ortho*-Ethoxy anethole
2646 *6*-Ethoxy-*meta*-anol
1135 .... *para*-Ethoxy benzaldehyde
1335 Ethoxybenzol
2018 Ethoxy-*iso*-chavibetol
611 *1*-Ethoxy-*4*-chlorobenzene
576 *2*-Ethoxy-*para*-cymene
2946 *3*-Ethoxy-*para*-cymene
2779 *1*-Ethoxy-*2,3*-dihydroxybenzene
2710 Ethoxydihydro trimethylquinoline
1282 *3*-Ethoxy-*3,7*-dimethyl-*1,6*-octadiene
906 Ethoxy ethane
1221 *2*-Ethoxy ethanol
1266 *ortho*-Ethoxy hexylbenzoate
1363 *3*-Ethoxy-*4*-hydroxybenzaldehyde
1721 *1*-Ethoxy-*4*-hydroxybenzene
2646 *1*-Ethoxy-*2*-hydroxy-*4*-propenylbenzene
2704 *1*-Ethoxy-*2*-hydroxy-*4*-propylbenzene
1232 *1*-Ethoxy-*2*-methoxy-*4*-allylbenzene
1233 *1*-Ethoxy-*2*-methoxy-*4*-propenylbenzene
2012 *ortho*-Ethoxy methylbenzoate
713 *4*-Ethoxy-*1*-methylbenzol
2301 *2*-Ethoxy naphthalene
1136 .... *ortho*-Ethoxy phenol
1721 *para*-Ethoxy phenol
2168 *N*-(*para*-Ethoxyphenyl)-*N*-methylurea
1125 *para*-Ethoxy phenylurea
1233 *2*-Ethoxy-*5*-propenylanisole
90 *para*-Ethoxy propenylbenzene
1231 *alpha*-Ethoxypropionic esters
1363 *3*-Ethoxy protocatechu aldehyde
2013 Ethoxy resocyanin
2921 *1*-Ethoxy tetralin
712 *meta*-Ethoxy toluene
1137 .... Ethyl acetate
549 Ethyl acetic acid
1138 .... Ethyl acetoacetate
2226 Ethyl acetone
1139 .... *para*-Ethyl acetophenone
1140 .... Ethyl acetosuccinate
1138 Ethyl acetyl acetate
1139 *4*-Ethyl-*1*-acetylbenzene
1348 Ethyl acetyl formate
1163 Ethyl-*alpha*-acetyl hydrocinnamate
1333 Ethyl acetyl phenol
1163 Ethyl-*2*-acetyl-*3*-phenylpropionate
1141 .... Ethyl aconitate
1142 .... Ethyl acrylate
1143 .... Ethyl adipate
1144 .... Ethyl alcohol (see also 1424)
3 Ethyl aldehyde
1145 .... Ethyl-*alpha*-allyl acetoacetate
1154 Ethyl-*ortho*-aminobenzoate
1230 *2*-Ethylamino ethylbenzoate
2402 Ethyl-*n*-amylcarbinol
1146 .... Ethyl-*iso*-amylcarbinol
2406 Ethyl-*n*-amylcarbinyl acetate
1147 .... Ethyl-*iso*-amyl carbinyl acetate
2413 Ethyl-*n*-amylcarbinyl-*iso*-butyrate
2059 Ethyl-*n*-amylcarbinyl formate
2434 Ethyl-*n*-amylcarbinyl phenylacetate
1148 .... Ethyl amyl ketone
1149 .... Ethyl-*iso*-amyl ketone
1150 .... Ethyl amyl methyl glycidate
1151 .... Ethyl-*iso*-amyl pyruvate
1688 "Ethyl anethole" (so-called)
1152 .... Ethyl angelate
1153 .... Ethyl anisate
1285 Ethyl-*ortho*-anisate
1288 Ethyl anisyl glycidate
1154 .... Ethyl anthranilate
1155 .... Ethyl asparaginate
1135 "Ethyl Aubepine"
1156 .... Ethyl benzaldehyde
1157 .... Ethyl benzene
1158 .... Ethyl benzilate
1159 .... Ethyl benzoate
1157 Ethyl benzol
1160 .... Ethyl benzoxyacetate
1161 .... Ethyl benzoyl acetate
1162 .... *para*-Ethyl benzyl acetate
1163 .... Ethyl benzyl acetoacetate
1164 .... *N*-Ethyl benzyl anthranilate

1165 .... *alpha*-Ethyl benzyl butyrate
309 Ethyl benzyl-*gamma*-butyrolactone
1166 .... Ethyl benzyl carbinol
1167 .... Ethyl benzyl carbinyl acetate
2481 *5*-Ethyl-*2*-benzyl-*1,3*-dioxolan
1168 .... Ethyl benzyl ether
1177 *2*-Ethyl butanal
1178 Ethyl butanoate
1179 Ethyl-*iso*-butanoate
1169 *2*-Ethyl butanol acetate
2014 *3*-Ethyl-*2*-butanone
1196 Ethyl-*2*-butenoate
1283 Ethyl-*iso*-butenoate
1746 Ethyl butenyl acetate
1169 .... *2*-Ethyl butyl acetate
310 Ethyl butyl acetic acid, benzylester
1252 *2*-Ethyl-*3*-butylacrolein
1503 Ethyl butyl carbinol
1170 .... Ethyl-*iso*-butylcarbinyl-*iso*-butyrate
1171 .... Ethyl butyl cyclohexyl caproate
1172 .... Ethyl-*secondary*-butylether
1173 .... Ethyl-*n*-butyl ketone
1174 .... Ethyl-*tertiary*-butyl ketone
1175 .... Ethyl butyl malonate
1176 .... Ethyl butyl phenoxyacetate
1177 .... *2*-Ethyl butyraldehyde
1178 .... Ethyl butyrate
1179 .... Ethyl-*iso*-butyrate
1180 .... *2*-Ethyl butyric acid
1180 *alpha*-Ethyl butyric acid
79 *2*-Ethylbutyric acid, allylester
1181 .... Ethyl butyro butyrate
1590 *gamma*-Ethyl-*n*-butyrolactone
1181 Ethyl-*alpha*-butyryl butyrate
1181 Ethyl-*alpha*-butyryl-*iso*-butyrate
1182 .... Ethyl butyryl lactate
1182 Ethyl-*alpha*-butyryl lactate
1208 Ethyl caprate
1208 Ethyl caprinate
1183 .... Ethyl caproate
80 *2*-Ethylcaproic acid, allylester
1257 *alpha*-Ethylcaproic aldehyde
1184 .... Ethyl caproyl caproate
1184 Ethyl caproyl hexoate
1185 .... Ethyl caprylate
2660 Ethyl carbinol
1141 Ethyl-*2*-carboxyglutaconate
576 Ethyl carvacrol
1136 Ethyl catechol
1325 Ethyl cetylate
90 Ethyl chavicol
1186 .... Ethyl chloracetate
1187 .... Ethyl chrysanthemumate
1188 .... Ethyl cinnamate
1188 Ethyl-*trans*-cinnamate
1189 .... *alpha*-Ethyl cinnamic aldehyde
1190 .... Ethyl citral
2990 Ethyl citrate
1191 .... Ethyl citronellate
1192 .... Ethyl citronellol
1004 "Ethyl citronellol" (see also 1246 and 1960)
682 Ethyl citronellyl acetal
1193 .... Ethyl citronellyl oxalate
1347 Ethyl coumalin
1194 .... *5*-Ethyl coumarin
1194 *6*-Ethyl coumarin
1195 .... Ethyl-*para*-cresyl acetal
1196 .... Ethyl crotonate
1196 Ethyl-*alpha*-crotonate
1197 .... Ethyl cyclocitrylidene acetate
1198 .... Ethyl-*beta*-cyclogeraniate
1199 .... Ethyl cyclohexane acetate
1200 .... Ethyl cyclohexane propionate
1201 .... *para*-Ethyl cyclohexanol
1202 .... Ethyl cyclohexyl acetate (see also 1199)
1203 .... Ethyl cyclohexyl butyrate
1203 Ethyl cyclohexyl-*iso*-butyrate
1204 .... Ethyl cyclohexyl propionate (see also 1200)
1205 Ethyl cyclopentenoate
1205 .... Ethyl cyclopentenyl acetate
1206 .... Ethyl decahydro-*beta*-naphthylacetate
914 Ethyl decane dioate
1208 Ethyl decanoate
1207 .... Ethyl decin carbonate
1208 .... Ethyl decylate (see also 1321)
1209 .... Ethyl decyl ether
1207 Ethyl dec-*1*-yne-*1*-carboxylate
1313 Ethyl-*2*-decynoate
904 Ethyl diethylene glycol
1340 Ethyl dihydrocinnamate
1152 Ethyl-*cis*-*2,3*-dimethylacrylate
1356 Ethyl-*trans*-*2,3*-dimethylacrylate
1210 .... Ethyl-*2,4*-dimethyl-*1,3*-dioxolane-*2*-acetate
1211 .... *para*-Ethyl-*alpha*-*alpha*-dimethyl hydrocinnamic aldehyde
1733 Ethyl-*N*-*3,7*-dimethyl-*7*-hydroxy-octyliden-anthranilate
1245 Ethyl-*3,7*-dimethyl-*2,6* (and -*2,7*)-octadienoate
1211 *para*-Ethyl-*alpha*-*alpha*-dimethyl phenylpropylaldehyde
1492 *3*-Ethyl-*2,4*-dimethylpyrrole
1293 Ethyl-*beta*-*para*-dimethyl-*1:2:3:6*-tetrahydrophenylpropionate
1158 Ethyl diphenylglycolate
1212 .... Ethyl-*2,4*-di-*iso*-propyl phenylglycidate
1213 .... *3a*-Ethyl-dodecahydro-*6,6,9a*-trimethylnaphtho-(*2,1*-*b*)-furan
1277 Ethyl dodecanoate (see also 1321)
1277 Ethyl dodecylate
1360 Ethyl dodecynoate
1216 Ethylene acetate
1214 .... Ethylene brassylate
53 Ethylene carboxylic acid
2854 Ethylene diamine tetra-acetate
1828 *cis*-*1,2*-Ethylene dicarboxylic acid
1411 *trans*-*alpha*-*beta*-Ethylene-*1,2*-dicarboxylic acid
909 Ethylene-*cis*-dicarboxylic acid, diethylester
1215 .... Ethylene glycol
1227 Ethylene glycol decane dioate
1216 .... Ethylene glycol diacetate
1217 .... Ethylene glycol di-monobromacetate

1218 .... Ethylene glycol di-thioglycolate
2991 Ethylene glycol-*bis*-*2*-hydroxyethylether
1219 .... Ethylene glycol monoallyl ether
1220 .... Ethylene glycol monobutylether acetate
1221 .... Ethylene glycol monoethyl ether
1222 .... Ethylene glycol monomethyl ether
1223 .... Ethylene glycol monophenyl ether
2465 Ethylene glycol monophenylether, acetate
2466 Ethyleneglycol monophenylether, *iso*-butyrate
2467 Ethyleneglycol monophenylether, propionate
2468 Ethyleneglycol monophenylether, *iso*-valerate
1224 .... Ethyleneglycol monopropyl ether
1224 Ethyleneglycol mono-*iso*-propylether
1225 .... Ethylene glycol mono-thioglycolate
1228 Ethyleneglycol nonane-dicarboxylate
1227 Ethyleneglycol-sebacic acid, cyclic ester
1226 .... Ethylene oxide
1227 .... Ethylene sebacate
1214 Ethylene tridecane dioate
1228 .... Ethylene undecandioate
1214 Ethylene undecane dicarboxylate
1290 Ethyl-*2*,*3*-epoxy-*3*,*6*-dimethylhexanoate
1298 Ethyl-*2*,*3*-epoxy-*3*,*7*-dimethyl-*6*-octenoate
1366 Ethyl-*alpha*-*beta*-epoxy-*beta*-(*2*,*4*-dimethylphenyl)-propionate
1212 Ethyl-*alpha*-*beta*-epoxy-*beta*-(*2*,*4*-di-*iso*-propylphenyl)-propionate
1316 Ethyl-*2*,*3*-epoxy dodecanoate
1296 Ethyl-*2*,*3*-epoxy-*3*-methyldecanoate
1303 Ethyl-*2*,*3*-epoxy-*3*-methyldodecanoate
1302 Ethyl-*2*,*3*-epoxy-*3*-methyl-*3*-(*para*-methoxyphenyl)-propionate
1309 Ethyl-*alpha*-*beta*-epoxy-*alpha*-methyl-*beta*-(*para*-methylphenyl)-propionate
1299 Ethyl-*2*,*3*-epoxy-*3*-methylnonanoate
1150 Ethyl-*2*,*3*-epoxy-*2*-methyloctanoate
1306 Ethyl-*alpha*-*beta*-epoxy-*beta*-methyl phenylpropionate
1307 Ethyl-*alpha*-*beta*-epoxy-*beta*-(*para*-methylphenyl)-propionate
1315 Ethyl-*2*,*3*-epoxy-*4*-methyl tridecanoate
1781 Ethyl-*2*,*3*-epoxy-*3*-methyl-*5*-(*2*,*6*,*6*-trimethyl-*2*-cyclohexenyl)-*4*-pentenoate
1339 Ethyl-*alpha*-*beta*-epoxy-*beta*-phenylpropionate
2024 Ethyl-*2*,*3*-epoxy-*3*-(*para*-tolyl)-propionate
906 Ethyl ether
1229 Ethyl-*ortho*-ethoxybenzoate
1229 .... Ethyl-*beta*-ethoxy salicylate
1230 .... Ethyl-*N*-ethyl anthranilate
1231 .... Ethyl ethyl lactate
1232 .... Ethyl eugenol
1233 .... Ethyl-*iso*-eugenol
1234 .... Ethyl everninate
1235 .... Ethyl formate
1235 Ethyl formiate
2654 Ethyl formic acid
1236 .... *2*-Ethyl furan
1240 Ethyl-*2*-furan carboxylate
1237 .... Ethyl-*2*-furan propionate
1238 .... *alpha*-Ethyl furfuracrolein
1239 .... Ethyl furfurhydracrylate
1242 Ethyl furfuryl alcohol
1244 Ethyl furfuryl ethylene lactate
1237 Ethyl furfuryl hydracrylate (see also 1244)
1240 .... Ethyl furoate
1238 *2*-Ethyl-*3*-furylacrolein
1238 *alpha*-Ethyl-*2*-furylacrolein
1241 .... *alpha*-Ethyl furyl acrylate
1242 .... Ethyl-*2*-furyl carbinol
1243 .... Ethyl furyl glycidate
1239 Ethyl furyl hydracrylate
1244 .... Ethyl furyl hydroxy acrylate
1239 Ethyl furyl-*beta*-hydroxypropionate
1237 Ethyl furyl propionate
1245 .... Ethyl geranate
1245 Ethyl geraniate
1246 .... Ethyl geraniol
1004 "Ethyl geraniol" (see also 1192 and 2035)
1247 .... Ethyl geranoxy acetate
1248 .... Ethyl geranyl acetone
1248 *6*-Ethyl geranyl acetone
1249 .... Ethyl geranyl ether
1221 Ethyl glycol
1250 .... Ethyl glycolate
1251 .... *4*-Ethyl guaiacol
1358 Ethyl hendecanoate
1359 Ethyl-*10*-hendecenoate
1252 .... *2*-Ethyl-*2*-heptenal
1253 .... Ethyl heptenone
1254 .... Ethyl heptin carbonate
1255 .... Ethyl heptoate (see also 1321)
1275 Ethyl heptoyl acetate
1255 Ethyl heptylate
1256 .... Ethyl heptyl ether
1261 Ethyl heptynoate
1305 Ethyl-*iso*-heptynoate
1325 Ethyl hexadecanoate
1351 Ethyl-*2*,*4*-hexadienoate
1199 Ethyl hexahydrophenylacetate
1200 Ethyl hexahydro phenylpropionate
1257 .... *2*-Ethyl hexanal
1258 .... Ethyl hexane diol
1259 .... *2*-Ethylhexane-*1*,*3*-diol monosalicylate
1183 Ethyl-*n*-hexanoate
1263 *2*-Ethylhexanoic acid (see also 2400)
1260 .... *2*-Ethyl hexanol
1262 *2*-Ethyl hexanyl acetate
1261 .... Ethyl hexin carbonate
1183 Ethyl hexoate
1262 .... *2*-Ethyl hexyl acetate (see also 2408)
1263 .... *2*-Ethyl hexyl acetic acid
1263 *2*-Ethyl-*2*-hexyl acetic acid

1264 .... Ethyl-*2*-hexyl acetoacetate
1265 .... *2*-Ethyl hexyl acrylate
1260 *2*-Ethyl hexyl alcohol
1183 Ethyl hexylate
2349 Ethyl hexyl carbinol
2354 Ethyl hexyl carbinyl acetate
1258 Ethyl hexylene glycol
1926 Ethyl-*iso*-hexyl ether
2351 Ethyl hexyl ketone
1266 .... Ethyl hexyl salicylate
1261 Ethyl-*n*--hex-*1*-yne carboxylate
1327 Ethyl hexynoate
1291 Ethyl-*iso*-hexynoate
1340 Ethyl hydrocinnamate
1267 .... *alpha*-Ethyl hydrocinnamic alcohol
1268 .... *alpha*-Ethyl hydrocinnamic aldehyde
1250 Ethyl hydroxyacetate
1350 Ethyl-*ortho*-hydroxybenzoate
1270 Ethyl-*3*-hydroxycaproate
1269 .... *alpha*-Ethyl-*2*-hydroxy cyclohexane acetic acid, *gamma*-lactone
1250 Ethyl hydroxy ethanoate
1270 .... Ethyl-*3*-hydroxy hexanoate
1234 Ethyl-*6*-hydroxy-*4*-methoxy-*ortho*-toluate
1234 Ethyl-*2*-hydroxy-*6*-methylanisate
1271 .... Ethyl-*alpha*-hydroxy-*alpha*-methylbutyrate
1349 Ethyl-*12*-hydroxy-*9*-octadecenoate
1272 .... Ethyl-*3*-hydroxy-*3*-phenylpropionate (see also 1161)
1231 *alpha*-Ethyl-*alpha*-hydroxypropionic acid, ethylester
1276 Ethyl-*alpha*-hydroxypropionate
1745 *3*-Ethyl-*2*-hydroxy-*4H*-pyran-*4*-one
5 Ethylidene di-*iso*-amylether
6 Ethylidene diethylether
9 Ethylidene dipropylether
1273 .... *beta*-Ethyl indole
1274 .... *alpha*-Ethyl ionone
765 "*iso*-Ethyl-*alpha*-ionone"
1781 Ethyl-*alpha*-ionone glycidate
2653 Ethyl ketone
1275 .... Ethyl-*beta*-ketopelargonate
1348 Ethyl ketopelargonate
1278 Ethyl-*gamma*-ketovalerate
1276 .... Ethyl lactate
1278 Ethyl laevulate
1277 .... Ethyl laurate
1277 Ethyl laurinate
1278 .... Ethal levulinate
1279 .... Ethyl linalool
1282 *3*-Ethyl linalool
1280 .... Ethyl linalyl acetate
1281 .... Ethyl linalyl acetate epoxide
1282 .... Ethyl linalyl ether
908 *dl*-Ethyl malate
909 Ethyl maleate
910 Ethyl malonate
450 Ethylmalonic acid, di-butylester
1355 Ethyl mercaptoacetate
1283 .... Ethyl methacrylate
910 Ethyl methane dicarboxylate
1235 Ethyl methanoate
1284 .... Ethyl-*alpha*-methoxybenzoate
1285 .... Ethyl-*ortho*-methoxybenzoate
1135 Ethyl-*para*-methoxybenzoate
1286 .... Ethyl-*ortho*-methoxy benzylether
1287 .... Ethyl-*para*-methoxycinnamate
1288 .... Ethyl-*para*-methoxy-*beta*-phenyl glycidate
1887 Ethyl-*ortho*-methoxy phenylketone
1941 Ethyl methyl acetic acid
1283 Ethyl-*alpha*-methylacrylate
1302 Ethyl methyl anisyl glycidate
1289 .... Ethyl-*N*-methyl anthranilate
1152 Ethyl-*cis*-*2*-methylbutenoate
1356 Ethyl-*trans*-*2*-methyl-*2*-butenoate
2019 *alpha*-Ethyl-*alpha*-methyl butenylacetone
1290 .... Ethyl methyl-*iso*-butyl glycidate
1291 .... Ethyl-*3*-methyl-*n*-but-*1*-yne carbonate
1292 .... Ethyl-*2*-methylbutyrate
1362 Ethyl-*beta*-methylbutyrate
1152 Ethyl-*cis*-*2*-methylcrotonate
1356 Ethyl-*trans*-*2*-methylcrotonate
1293 .... Ethyl-*beta*-(*4*-methyl-*3*-cyclohexenyl)-butyrate
1294 .... Ethyl-*2*-methyl-*1*,*3*-dioxolane-*2*-acetate
1343 Ethyl-*3*,*4*-methylenedioxybenzoate
1295 .... Ethyl-*6*-methyl-*n*-hept-*5*-en-*1*-yne carbonate
1297 Ethyl methyl heptin carbonate
1296 .... Ethyl methyl heptyl glycidate
1297 .... Ethyl-*6*-methyl-*n*-hept-*1*-yne carbonate
1298 .... Ethyl methyl-*iso*-hexenyl glycidate
1300 Ethyl methyl hexin carbonate
1299 .... Ethyl methyl hexyl glycidate
1300 .... Ethyl-*5*-methyl-*n*-hex-*1*-yne carbonate
2020 Ethyl methyl ketone
1301 .... Ethyl methyl lactate
1302 .... Ethyl-*beta*-methyl-*beta*-*para*-methoxyphenyl glycicate
1309 Ethyl methyl-*para*-methyl phenylglycidate
1303 .... Ethyl methyl nonyl glycidate
1297 Ethyl-*6*-methyl-*2*-octynoate
1304 .... Ethyl-2-methyl-2-pentenoate
1305 .... Ethyl-*4*-methyl-*n*-pent-*1*-yne carbonate
2021 Ethyl methyl phenyl carbinol
2022 Ethyl methyl phenyl carbinylacetate
1306 .... Ethyl methyl phenyl glycidate
1307 .... Ethyl-*para*-methyl-*beta*-phenyl glycidate
1283 Ethyl-*2*-methyl-*2*-propenoate
1308 .... *3*-Ethyl-*4*-methyl pyridine
1285 "Ethyl methyl salicylate"
1309 .... Ethyl methyl-*para*-tolyl glycidate
1186 Ethyl monochloroacetate
1307 Ethyl-*para*-M.P.G.
1310 .... Ethyl myristate
2301 Ethyl-*beta*-naphthylether
2301 Ethyl-*2*-naphthylether
1311 .... Ethyl nitrate and ethyl nitrite
1311 "Ethyl nitrate spirits"

1312 .... Ethyl nonanoate
1314 Ethyl-*2*-nonenoate
1295 Ethyl-*iso*-nonenynoate
1313 .... Ethyl nonin carbonate
1312 Ethyl nonylate
1314 .... Ethyl nonylenate
1315 .... Ethyl nonyl ethyl glycidate
1316 .... Ethyl nonyl glycidate
1313 Ethyl nonyne carboxylate
1297 Ethyl-*iso*-nonynoate
1317 Ethyl-*2*-nonynoate
1352 Ethyl octadecanoate
1322 Ethyl-*9*-octadecenoate
1353 Ethyl octane dioate
1185 Ethyl octanoate
1317 .... Ethyl octin carbonate
1185 Ethyl octoate (see also 1321)
1185 Ethyl octylate
1318 Ethyl-*2*-octyl-*2*-butenoate
1318 .... Ethyl octyl crotonate
1320 Ethyl octyl glycolate
1319 .... Ethyl octyl ketone
1320 .... Ethyl octyl-*2*-oxyacetate
1317 Ethyl octyne carboxylate
1254 Ethyl-*2*-octynoate
1300 Ethyl-*iso*-octynoate
1321 .... Ethyl oenanthate (see also 1255)
1322 .... Ethyl oleate
1323 .... Ethyl orthoformate
912 Ethyl oxalate
906 Ethyl oxide
1138 Ethyl oxobutanoate
1348 Ethyl-*2*-oxopropanoate
1324 .... Ethyl oxyhydrate
1349 Ethyl oxyoleate
1745 "Ethyl Palatone"
1325 .... Ethyl palmitate
1312 Ethyl pelargonate
1326 .... Ethyl pentadecanoate
1326 Ethyl pentadecylate
1361 Ethyl pentanoate
1362 Ethyl-*iso*-pentanoate
1327 .... Ethyl pentin carbonate
1327 Ethyl-*n*-pent-*1*-yne carbonate
1328 .... *ortho*-Ethyl phenol
1329 .... *para*-Ethyl phenol
1330 .... Ethyl phenoxy acetate
1331 .... *para*-Ethyl phenylacetaldehyde
1332 .... Ethyl phenylacetate
1333 .... *para*-Ethyl phenyl acetate
1188 Ethyl-*beta*-phenylacrylate
1334 .... Ethyl phenylbutyrate
1334 Ethyl-*4*-phenylbutyrate
2520 Ethyl phenyl carbinol
2521 Ethyl phenyl carbinyl acetate
1165 Ethyl phenyl carbinyl-*n*-butyrate
1335 .... Ethyl phenyl ether
1336 .... Ethyl phenylethoxy acetate
1337 .... Ethyl phenylethyl acetal
1167 *alpha*-Ethyl-*beta*-phenylethyl acetate
1166 *alpha*-Ethyl phenylethyl alcohol
2526 Ethyl phenylethyl carbinol
2527 Ethyl phenylethyl carbinyl acetate
1338 .... Ethyl phenylethyl ether
1339 .... Ethyl phenyl glycidate
2023 Ethyl phenyl glycidic acid, methyl-ester
2656 Ethyl phenyl ketone
1267 *alpha*-Ethyl-*beta*-phenylpropanol
1189 *2*-Ethyl-*3*-phenyl-*2*-propenal-*1*
1188 Ethyl-*3*-phenylpropenoate
1340 .... Ethyl-*3*-phenylpropionate
1268 *2*-Ethyl-*beta*-phenylpropionic aldehyde
1341 .... Ethyl phenylpropoxy acetate
913 Ethyl phthalate
1342 "Ethyl piperonyl acetate"
1342 .... Ethyl piperonyl acrylate
1343 .... Ethyl piperonylate
1342 "Ethyl piperonylidene acetate"
910 Ethyl propane dioate
1344 Ethyl propanoate
1141 Ethyl-*1*-propene-*1*,*2*,*3*-tricarboxylate
1142 Ethyl propenoate
1351 Ethyl-*2*-propenylacrylate
1344 .... Ethyl propionate
1345 .... *alpha*-Ethyl-*para*-*iso*-propyl cinnamic aldehyde
1258 *2*-Ethyl-*3*-propyl-*1*,*3*-propanediol
1363 Ethyl protal
1346 .... *4*-Ethyl pyridine
1240 Ethyl pyromucate
1347 .... *5*-Ethyl-*alpha*-pyrone
1347 *5*-Ethyl-*2*-pyrone
1348 Ethyl pyro-racemate
1348 .... Ethyl pyruvate
1349 .... Ethyl ricinoleate
1350 .... Ethyl salicylate
1285 Ethyl salicylate, methylether
914 Ethyl sebacate
1351 .... Ethyl sorbate
1352 .... Ethyl stearate
1353 .... Ethyl suberate
915 Ethyl succinate
916 Ethyl tartrate
1326 Ethyl tetradecane-*1*-carboxylate
1310 Ethyl tetradecanoate (see also 1321)
1354 .... *2*-Ethyl tetrahydrofuran
2930 *5*-Ethyl-*2*,*3*,*4*,*5*-tetramethyl-*2*-cyclohexen-*1*-one
2930 *5*-Ethyl-*3*,*4*,*5*,*6*-tetramethyl-*2*-cyclohexen-*1*-one
1354 *2*-Ethyl tetramethylene oxide
1355 .... Ethyl thioglycolate
1356 .... Ethyl tiglate
1332 Ethyl-*alpha*-toluate
713 Ethyl-*para*-tolylether
1307 Ethyl-*para*-tolylglycidate
1357 .... *alpha*-Ethyl-*2*,*2*,*6*-trimethyl-cyclohexane butyric aldehyde
1358 Ethyl undecanoate
1359 Ethyl-*10*-undecenoate
1358 .... Ethyl undecin carbonate
1359 .... Ethyl undecylate
1360 .... Ethyl undecylenate
1360 Ethyl undecyne carbonate
1207 Ethyl undecynoate
1361 .... Ethyl valerate
1362 .... Ethyl-*iso*-valerate

1361 Ethyl valerianate
1362 Ethyl-*iso*-valerianate
1363 .... Ethyl vanillin (commercial name)
1364 .... *iso*-Ethyl vanillin
1365 .... Ethyl vanillin (true chemical name)
1745 "Ethyl Veltol"
2454 Ethyl vinyl carbinol
2455 Ethyl vinyl carbinyl acetate
3093 Ethyl vinyl ether
1366 .... Ethyl xylyl glycidate
2643 Ethynyl carbinol
1133 *1*-Ethynyl cyclohexan-*1*-yl acetate
1363 Ethyvan
616 Eucalyptol
2630 Eucalyptus dives oil
2719 "Eucalyptus ketone"
2694 Eucalyptus polybractea (see also 2732 and 2733)
1052 Eudalene
2842 *alpha*-Eudesmene
1367 .... Eudesmol (see also 1052)
1368 .... Eudesmyl acetate
1369 Eugenic acid
1369 .... Eugenol
1370 .... *iso*-Eugenol
1370 *cis-iso*-Eugenol
2645 *ortho-iso*-Eugenol
1370 *trans-iso*-Eugenol
944 Eugenol M
14 Eugenol acetate
15 *iso*-Eugenol acetate
170 Eugenol amylether
171 *iso*-Eugenol amylether
284 Eugenol benzoate
285 *iso*-Eugenol benzoate
311 Eugenol benzylether
312 *cis-iso*-Eugenol benzylether
313 *trans-iso*-Eugenol benzylether
1372 Eugenol cinnamate
635 Eugenol cinnamylether
1232 Eugenol ethylether
1233 *iso*-Eugenol ethylether
1373 Eugenol formiate
1538 Eugenol heptylether
1539 *iso*-Eugenol heptylether
1662 *iso*-Eugenol hexylether
1371 .... Eugenol methyl acetal
2026 Eugenol methylether
2027 *iso*-Eugenol methylether
1375 Eugenol phenylacetate
1376 *iso*-Eugenol phenylacetate
2560 *iso*-Eugenol phenylether
14 Eugenyl acetate
284 Eugenyl benzoate
1372 .... Eugenyl cinnamate
1373 .... Eugenyl formate
1374 .... *iso*-Eugenyl formate
1375 .... Eugenyl phenylacetate
1376 .... *iso*-Eugenyl phenylacetate
1377 .... *beta*-Euionone
3069 "Eupyrin"
451 Everninic acid, *iso*-butylester
1234 Everninic acid, ethylester
2028 Everninic acid, methylester
811 "Exaltolide"
813 "Exaltone"
897 Exo-*3a*-*4*,*5*,*6*,*7*,*7a*-hexahydro-*4*,*7*-methanoindane-*2*-carboxaldehyde
1872 Exo-*3a*,*4*,*5*,*6*,*7*,*7a*-hexahydro-*5* (or-*6*) -methoxy-*4*,*7*-methanoindan-*2*-carboxaldehyde

**F**

3014 "Farenal"
1378 .... Farnesal
1379 .... Farnesene
1380 .... Farnesol
1381 .... Farnesyl acetate
1382 .... Farnesyl acetone
1383 .... Farnesylidene acetone
1387 Fenchanol
1384 .... Fenchene
1387 Fenchol
1385 .... Fenchone
1386 .... Fenchyl acetate
1387 .... Fenchyl alcohol
1388 .... Fenchyl benzoate
1389 .... Fenchyl-*n*-butyrate
1390 .... Fenchyl-*iso*-butyrate
2943 Fennel ("Dog Fennel")
126 Fermentation amylalcohol
1051 Fermine
13 Fernon
703 Ferula alcohol
702 Ferulaldehyde
3074 Ferulic methylketone
1391 .... Fixateur 404
1728 Fixol
1728 Fixonal
1534 "Fleuramone"
2191 "Fliedenol"
2189 "Fliedenol acetate" (see also 2958)
149 Flomine
2976 "Floranal"
2466 "Floranol"
149 Flosal
158 Floxin acetate
149 Floxine
159 Floxin formate
161 Floxin-*iso*-valerate
1392 .... *2*-Fluoro-*4*,*6*-dinitro-*1*,*3*-dimethyl-*5*-*tertiary*-butyl benzene
2485 "Foliacetal"
2237 "Folianthine"
2485 "Foliol Rosal"
2045 "Folione"
1703 "Foretine"
1397 Formal
1393 .... Formaldehyde-*iso*-amyl phenylethyl acetal
1394 .... Formaldehyde di-*iso*-amylacetal
1395 .... Formaldehyde dibutyl acetal
896 Formaldehyde di-cyclohexyl acetal
1396 .... Formaldehyde diethyl acetal
1397 .... Formaldehyde dimethyl acetal
1398 .... Formaldehyde di-propyl acetal
1399 .... Formaldehyde ethyl anisyl acetal
1400 .... Formaldehyde ethyl cinnamyl acetal
1401 .... Formaldehyde ethyl dimethyloctanyl acetal
1402 .... Formaldehyde ethyleneglycol acetal

1403 .... Formaldehyde ethyl hydroxycitronellyl acetal
1404 .... Formaldehyde ethyl phenylethyl acetal
1405 .... Formaldehyde ethyl "Rhodinyl" acetal
1406 .... Formaldehyde ethyl terpinyl acetal
1407 .... Formaldehyde methyl phenylethyl acetal
1408 .... Formaldehyde phenylethyl cyclohexyl acetal
1409 .... Formaldehyde phenylethyleneglycol acetal
1410 .... Formic acid
1235 Formic ether
1713 Formonitrile
1413 *2*-Formyl furan
811 "Fortolide"
2299 "Fragarol"
1306 "Fraise"
1306 "Fraiseol"
1760 "Frambinone, cryst."
248 "Frambinone methylether"
1294 "Fructone"
1210 "Fructone B"
2041 "Fructurol"
77 "Fruit ketone"
1411 .... Fumaric acid
1421 Furacrolein
1413 Fural
1413 *2*-Furaldehyde
1412 .... Furan
1420 Furanacetaldehyde
1421 *2*-Furanacrolein
1413 Furan-*alpha*-aldehyde
1413 Furan-*2*-aldehyde
174 *2*-Furanbutyric acid, *iso*-amylester
1413 *2*-Furancarbonal
1418 Furan-*alpha*-carboxylic acid
1418 Furan-*2*-carboxylic acid
178 Furan-*alpha*-carboxylic acid, *n*-amylester
458 Furan-*alpha*-carboxylic acid, *n*-butylester
1542 Furan-*alpha*-carboxylic acid, *n*-heptylester
2033 Furan-*alpha*-carboxylic acid, methylester
2709 Furan-*alpha*-carboxylic acid, *n*-propylester
1417 *2*-Furan methane thiol
175 *2*-Furanpropionic acid, *iso*-amylester
1421 "Furfuracrolein"
1413 .... Furfural
1414 .... Furfural acetone
1416 Furfuralcohol
1413 Furfuraldehyde
1412 Furfuran
1413 "Furfurol"
1415 .... Furfuryl acetate
1414 "Furfuryl acetone"
1416 .... Furfuryl alcohol
918 Furfuryl disulfide
1414 Furfurylidene acetone
1238 *2*-Furfurylidene butyraldehyde
176 *alpha*-Furfurylidene heptanal
1541 *alpha*-Furfurylidene nonanal
1417 .... *alpha*-Furfuryl mercaptan
1418 .... *2*-Furoic acid
178 *2*-Furoic acid, *n*-amylester
1413 "Furol"
1419 .... Furoyl acetone
1420 .... *2*-Furyl acetaldehyde
1423 Furyl acetone
1421 *beta*-*2*-Furyl acraldehyde
1421 .... Furyl acrolein
1422 .... *2*-Furyl allylalcohol
1422 *beta*-Furyl allylalcohol
1419 *1*-(*2'*-Furyl-)-*1*,*3*-butandione
1414 *4*-(*2*-Furyl)-*3*-buten-*2*-one
1416 *alpha*-Furyl carbinol
1416 *2*-Furyl carbinol
1415 *2*-Furyl carbinyl acetate
1243 *beta*-*2*-Furyl-*alpha*-*beta*-epoxy ethylpropionate
1242 *2*-Furyl ethyl carbinol
1413 *alpha*-Furyl formaldehyde
1414 *2*-Furylidene acetone
1417 *2*-Furyl methane thiol
1930 "Furyl methyl-*iso*-butylketone"
1423 .... (*2*-Furyl)-*3*-propanone
1421 *beta*-*2*-Furyl propenal
456 *beta*-Furylpropionic acid, *n*-butylester
119 Fusel
126 Fusel amylalcohol
143 Fusel amylcaproate
1424 .... Fusel oil

**G**

1793 *4*-(*beta*-*D*-Galactopyranosido)-*D*-glucose
1581 "Galaxolide"
2513 "Gallicol"
2871 "Gallotannic acid"
1742 Gallusaldehyde-*3*,*5*-dimethylether
135 "Gardenia oxide" (see also 1644)
2566 "Gardeniol I"
2176 "Gardeniol II"
2176 "Gardenol"
649 Geranial
1425 .... Geranic acid
1451 Geranic acid, nitrile
1426 .... Geraniol
1427 .... *iso*-Geraniol
1009 Geraniolene
1081 "Geranium crystals"
2809 "Geranium oxides"
1451 Geranonitrile
1428 .... Geranoxy acetaldehyde
1429 .... Geranoxy acetaldehyde diethyl acetal
1452 Geranoxy acetic acid
1247 Geranoxyacetic acid, ethylester
2036 Geranoxyacetic acid, methylester
1430 .... Geranyl acetate
1431 .... Geranyl acetoacetate
1432 .... Geranyl acetone
1433 .... Geranyl anthranilate
1434 .... Geranyl benzoate
1443 Geranyl-*2*-butenoate
1435 .... Geranyl-*iso*-butyraldehyde
1436 .... Geranyl butyrate

1437 .... Geranyl-*iso*-butyrate
1438 .... *alpha*-Geranyl-*gamma*-byturolactone
1439 .... Geranyl-*iso*-butyronitrile
1440 .... Geranyl caproate
1441 .... Geranyl caprylate
1442 .... Geranyl cinnamate
1443 .... Geranyl crotonate
1443 Geranyl-*alpha*-crotonate
1444 .... Geranyl ethoxyacetate
1445 .... Geranyl ethylcarbonate
2038 Geranyl-*alpha*-ethylcrotonate
1249 Geranyl ethylether
1446 .... Geranyl formate
1447 .... Geranyl furoate
2613 "Geranyl geraniol" (hexahydro-)
1448 .... Geranyl heptoate
1448 Geranyl heptylate
1544 Geranyl heptylether
1440 Geranyl hexanoate
1449 .... Geranyl linalool
1450 .... Geranyl methoxy acetate
2035 Geranyl methylether (see also 2037)
2038 Geranyl methyl ethyl acrylate
769 Geranyl methyl ketone
2038 Geranyl methyl tiglate
1451 .... Geranyl nitrile
1453 Geranyl nonanoate
1453 Geranyl nonylate
1441 Geranyl octoate
1441 Geranyl octylate
1428 Geranyl oxyacetaldehyde (see also 688)
1452 .... Geranyl oxyacetic acid
1453 .... Geranyl pelargonate
1454 .... Geranyl phenylacetate
1442 Geranyl-*3*-phenylpropenoate
1455 .... Geranyl phthalate
1456 .... Geranyl propionate
1457 .... Geranyl-*iso*-propoxyacetate
1439 Geranyl-*iso*-propylcyanide
1447 Geranyl pyromycate
1458 .... Geranyl salicylate
1459 .... Geranyl tiglate
1460 .... Geranyl valerate
1461 .... Geranyl-*iso*-valerate
1462 .... Geranyl vinyl ether
2976 "Gerindol"
1463 Germacrol
1463 .... Germacrone
2854 "Giltex"
2845 Ginger
2845 Gingerol
2835 Ginseng
789 "Givmenthe"
2485 "Gladioline"
2860 *dextro*-Glucitol
1464 .... Glucose
2868 "Glucose octa-acetate"
1465 .... Glucose penta-acetate
2812 "Gluside"
2273 "Glutacyl"
1466 .... *laevo*-Glutamic acid
1466 *L-dextro*-Glutaminic acid
907 *L-alpha*-Glutaminic acid, diethylester
1466 Glutaminol
1466 Glutaton
2273 "Glutavene"
1467 .... Glycerin
1467 Glycerol
474 Glycerol-*1*,*2*-butylacetal (cyclic)
1468 .... Glycerol dimethylketal
871 Glyceryl diacetate
2271 Glyceryl monoacetate
1470 Glyceryl mono-octadecanoate
1469 .... Glyceryl mono-oleate
1470 Glyceryl monopalmitate
1470 .... Glyceryl monostearate
2971 Glyceryl triacetate
2973 Glyceryl tributyrate
2004 "Glycidate M-116"
1215 Glycol
1216 Glycol diacetate
634 Glycolic ethylether, cinnamylester
1402 Glycol formal
2464 Glycolic acid, phenylether
1055 Glycoline
1402 Glycol methylal
1402 Glycol methylene ether
1227 Glycol sebacate
1471 Glycyrrhetinic acid glucoside, ammonium salt
1471 .... Glycyrrhizin, ammoniated
1464 Grape sugar
2514 "Graposynth"
1136 Guaethol
1472 .... Guaiacol
1473 .... Guaiacol allylether
1474 .... Guaiacol ethylether
1480 "Guaiacwood acetate"
1475 .... Guaiacyl acetate
1476 .... Guaiacyl benzoate
1477 .... Guaiacyl phenylacetate
1478 .... Guaiene
1479 .... Guaiol
1480 .... Guaiyl acetate
1481 .... Guaiyl butyrate
1482 .... Guaiyl formate
1483 .... Guaiyl phenylacetate (see also 1477)
558 Guaranine

**H**

702 "Hadromal"
2854 "Hagan phosphate"
113 "Hartshorn"
1719 "Hazeltone"
1653 "H.C.A."
56 "Helenin"
13 "Helional" (see also 2110)
13 "Heliopon"
1488 "Heliotrope blanc"
2632 Heliotropic acid
518 Heliotropic acid, *iso*-butylester
1484 .... Heliotropine
1485 .... Heliotropine diethyl acetal
1486 .... Heliotropine dimethyl acetal
1692 Heliotropine, liquid
1487 .... Heliotropyl acetate
1488 .... Heliotropyl acetone
1489 .... Heliotropyl alcohol
1490 .... Heliotropyl-*iso*-butyrate
2631 Heliotropyl ethylcarbonate

1491 .... Heliotropylidene acetaldehyde
1488 Heliotropylidene acetone
2633 Heliotropylidene diacetate
1492 .... *iso*-Hemopyrrole
3028 Hendecanal
3031 *1*-Hendecanol
3024 *1,4*-Hendecanolide
2140 *2*-Hendecanone
3034 Hendecen-*9*-al
3035 Hendecen-*10*-al
3049 Hendecen-*1*-oic acid-*11*
3041 *10*-Hendecenyl acetate
2262 Hendecyl methyl ketone
2863 Heptadecane-*1*-carboxylic acid
2680 *n-alpha*-Heptalactone
1504 *gamma*-Heptalactone
1494 Heptaldehyde
1495 Heptaldehyde diethyl acetal
1496 Heptaldehyde dimethyl acetal
986 Heptaldehyde-*2,2*-dimethyl-*1,3*-propanediol (cyclic) acetal
1497 Heptaldehyde di-*iso*-propyl acetal
1660 Heptaldehyde glycol acetal
1549 Heptaldehyde-methylanthranilate
1675 Heptaldehyde-propyleneglycol acetal
1493 .... Heptamethylene carbonate
1494 .... *n*-Heptanal
1495 .... Heptanal diethyl acetal
1496 .... Heptanal dimethyl acetal
1497 .... Heptanal di-*iso*-propyl acetal
1660 Heptanal-ethyleneglycol (cyclic) acetal
1498 .... Heptanal glyceryl acetal
1675 Heptanal-*1,2*-propanediol (cyclic) acetal
1499 .... Heptane
47 *2,3*-Heptanedione
1513 Heptanoic acetate
1500 .... Heptanoic acid
1494 Heptanoic aldehyde
1501 .... *1*-Heptanol
1502 .... *2*-Heptanol
1503 .... *3*-Heptanol
1088 *4*-Heptanol
2680 Heptanolide
1504 .... Heptanolide-(*4,1*)
1905 *2*-Heptanone
1173 *3*-Heptanone
1090 *4*-Heptanone
1514 *2*-Heptanyl acetate
1505 .... *cis-4*-Hepten-*1*-al
388 *beta-iso*-Heptenal
1506 .... *trans-2*-Hepten-*1*-al
1507 .... *trans-4*-Heptenal
1508 .... *cis-4*-Hepten-*1*-al diethyl acetal
1506 *alpha-beta*-Heptenoic aldehyde
1509 .... *4*-Hepten-*1*-ol
472 *3*-Hepten-*2*-one
1510 .... *cis-4*-Heptenyl acetate
820 Heptenyl acrolein
1511 .... *cis-4*-Heptenyl-*iso*-butyrate
2268 "*iso*-Heptenyl lactone"
1500 Heptoic acid
1512 .... *n*-Heptoxy acetic acid
1559 *n*-Heptoxy benzene
1513 .... Heptyl acetate
1514 .... *secondary*-Heptyl acetate
1515 .... *iso*-Heptyl acetate
1516 .... Heptyl acetoacetate
2146 Heptyl acetone
842 *3*-Heptyl acrolein
2129 *3-iso*-Heptyl acrolein
842 *trans-beta-n*-Heptyl acrolein
843 *3*-Heptyl acrylic acid
1501 *n-primary*-Heptyl alcohol
1502 *secondary*-Heptyl alcohol
1494 *n*-Heptyl aldehyde
1518 Heptyl-*ortho*-aminobenzoate
185 *n*-Heptyl-*iso*-amylether
1517 .... *n*-Heptyl anisate
1518 .... *n*-Heptyl anthranilate
1519 .... *n*-Heptyl benzoate
1520 .... Heptyl benzyl ether
1521 *n*-Heptyl-*n*-butanoate
1522 *n*-Heptyl-*iso*-butanoate
464 Heptyl butyl ether
465 *n*-Heptyl-*iso*-butyl ether
464 Heptyl butyl oxide
1521 .... *n*-Heptyl-*n*-butyrate
1522 .... Heptyl-*iso*-butyrate
1170 *secondary-iso*-Heptyl-*iso*-butyrate
1523 .... *alpha*-Heptyl-*gamma*-butyrolactone
3024 *gamma-n*-Heptyl-*gamma*-butyrolactone
1524 .... *n*-Heptyl caprate
1524 Heptyl caprinate
1525 .... *n*-Heptyl caproate
1526 .... *n*-Heptyl caprylate
2401 Heptyl carbinol
1528 Heptyl cinnamal
1527 .... *n*-Heptyl cinnamate
1528 .... *alpha-n*-Heptylcinnamic aldehyde
1529 .... Heptyl cinnamyl ether
1530 .... Heptyl citronellate
1531 .... *para*-Heptyl cyclohexanol
1532 .... *para*-Heptyl cyclohexanone
1533 .... *2-n*-Heptyl cyclopentanol
1534 .... *2-n*-Heptyl cyclopentanone
1535 .... Heptyl cyclopentenone
1524 Heptyl decanoate
1524 Heptyl decylate
1536 .... Heptyl decyl ether
1536 Heptyl decyl oxide
1522 *n*-Heptyl dimethylacetate
1550 Heptyl dodecanoate
1550 *n*-Heptyl dodecylate
1537 .... Heptyl dodecyl ether
919 *n*-Heptylether
1256 Heptyl ethyl ether
1538 .... Heptyl eugenol
1539 .... Heptyl-*iso*-eugenol
1540 .... Heptyl formate
1541 .... *alpha*-Heptyl furfuracrolein
1542 .... *n*-Heptyl furoate
1541 *alpha-n*-Heptyl-*beta-2*-furylacrolein
1543 .... Heptyl geraniate
1544 .... Heptyl geranyl ether
1544 Heptyl geranyl oxide
1545 *n*-Heptyl-*n*-heptanoate
1545 .... *n*-Heptyl heptoate

1545 Heptyl heptylate
1557 Heptyl hexadecanoate
1525 *n*-Heptyl-*n*-hexanoate
1525 Heptyl hexylate
1668 Heptyl hexyl ether
1562 *n*-Heptyl-*ortho*-hydroxybenzoate
1500 Heptylic acid
2356 Heptylidene acetaldehyde
1546 .... Heptylidene acetone
1547 .... *2-n*-Heptylidene cyclopentanone
1548 .... Heptylidene heptanal
1549 .... Heptylidene methylanthranilate
1549 "Heptylique"
2680 *alpha-n*-Heptyllactone
1550 .... Heptyl laurate
1551 .... Heptyl linalyl ether
149 "Heptyllis"
1540 *n*-Heptyl methanoate
1517 Heptyl-*para*-methoxybenzoate
2049 *2-n*-Heptyl-*2*-methylcyclopentan-*1*-one
2051 Heptyl methyl ether
1569 Heptyl methyl ethyl acetate
2052 Heptyl methyl ketone
1522 *n*-Heptyl-*2*-methylpropanoate
1552 .... Heptyl myristate
1553 Heptyl nonanoate
1553 .... *n*-Heptyl nonylate
1554 .... Heptyl nonyl ether
1554 Heptyl nonyl oxide
1556 Heptyl-*9*-octadecenoate
1526 Heptyl octanoate
1526 Heptyl octylate
1555 .... Heptyl octyl ether
1555 Heptyl octyl oxide
1556 .... *n*-Heptyl oleate
1516 Heptyl-*3*-oxobutanoate
1557 .... *n*-Heptyl palmitate
1553 Heptyl pelargonate
1568 Heptyl-*n*-pentanoate
1569 Heptyl-*iso*-pentanoate
1560 Heptyl phenethyl ether
1558 .... Heptyl phenylacetate
1559 .... Heptyl phenyl ether
1560 .... Heptyl phenylethyl ether
1559 Heptyl phenyl oxide
1561 Heptyl propanoate
1995 *2*-Heptylpropenoic acid, methylester
1561 .... Heptyl propionate
2713 *n*-Heptyl-*n*-propylether
2714 *n*-Heptyl-*iso*-propylether
2715 Heptyl propyl ketone
1542 *n*-Heptyl pyromucate
1562 .... Heptyl salicylate
1552 Heptyl tetradecanoate
1563 .... *2-(n*-Heptyl)-tetrahydrofuran
1558 Heptyl-*alpha*-toluate
1565 Heptyl undecanoate
1566 Heptyl undecenoate
1564 .... Heptyl undecenyl ether
1565 .... Heptyl undecylate
1566 .... Heptyl undecylenate
1567 .... Heptyl undecyl ether
1568 .... Heptyl valerate
1569 .... Heptyl-*iso*-valerate
1103 *n*-Heptyl-*delta*-valerolactone
1570 .... Hercolyn
2255 Herniarin
2162 "Hesperia"
1800 Hesperidene
3094 Hesperitol
1891 *iso*-Hesperitol
1571 .... Hexachloro ethane
2894 Hexadecamethylene carbonate
1572 .... Hexadecamethylenimine
1573 .... Hexadecanal
2447 Hexadecanoic acid
1574 .... Hexadecanol
923 Hexadecanolide
1574 *n*-Hexadecyl alcohol
1573 Hexadecyl aldehyde
2447 *n*-Hexadecylic acid
1575 .... *2,4*-Hexadienal
1576 .... Hexadiene
973 *1,5*-Hexadiene-*3,4*-diol
2858 *2,4*-Hexadienoic acid
1577 .... Hexadienol
1577 *2,4*-Hexadien-*1*-ol
1578 .... Hexadienyl-*iso*-butyrate
1579 .... Hexadienylidene acetone
36 Hexahydro acetophenone
773 Hexahydrobenzaldehyde diethyl acetal
774 Hexahydrobenzaldehyde dimethyl acetal
795 Hexahydro benzylacetate
796 Hexahydro benzylalcohol
798 Hexahydrobenzyl-*trans-2*-butenoate
797 Hexahydrobenzyl-*iso*-butyrate
798 Hexahydrobenzyl-*beta*-methacrylate
799 Hexahydro benzylpropionate
1980 Hexahydro-*para*-cresol ethylether
1976 Hexahydro-*ortho*-cresylacetate
1977 Hexahydro-*para*-cresylacetate
1836 Hexahydro-*para*-cymene
1171 Hexahydro diethyl phenylethyl caproate
1580 .... Hexahydro farnesal
2613 Hexahydro geranylgeraniol
2614 Hexahydro geranyllinalool
1581 .... *1,3,4,6,7,8*-Hexahydro-*4,6,6,7,8,8*-hexamethyl-cyclopenta-*gamma-2* benzopyran
2690 "Hexahydro homocuminic alcohol"
803 Hexahydro hydratropic alcohol
1582 .... *3a,4,5,6,7,7a*-Hexahydro-*4,7*-methano-*5*-indanol
1583 .... *3a,4,5,6,7,7a*-Hexahydro-*4,7*-methanoindene-*5*-(or-*6*-)-carboxaldehyde diethyl acetal
1584 .... *3a,4,5,6,7,7a*-Hexahydro-*4,7*-methanoindene-*5*-(or-*6*-)-methyl acetate
1585 .... *3a,4,5,6,7,7a*-Methanoinden-*5*-(or-*6*-)-yl-oxyacetaldehyde
1981 Hexahydro-*para*-methyl styrallyl-acetate
2334 Hexahydronitrobenzene
3015 Hexahydro-nor-farnesal
1586 .... *1,3,4,6,7,8*-Hexahydro-*4,6,6,8,8*-

pentamethyl cyclopenta-(*g*)-*2*-benzopyran
1587 .... *3,4,6,7,8,9*-Hexahydro-*4,6,6,9,9*-pentamethyl-*1H*-naphtho-(*2,3c*)-pyran
776 Hexahydrophenol
780 Hexahydro phenylacetaldehyde
772 Hexahydro phenylacetic acid
783 Hexahydro phenylbenzoate
1199 Hexahydro phenylethylacetate (see also 1202)
791 Hexahydro phenylethylalcohol
1203 Hexahydro phenylethyl-*n*-butyrate
1203 Hexahydro phenylethyl-*iso*-butyrate
1204 Hexahydro phenylethyl propionate
804 Hexahydro phenylpropylalcohol
557 *3,4,5,8,9,10*-Hexahydro-*4*-*iso*-propyl-*1,6*-dimethylnaphthalene
2724 Hexahydro-*para*-*iso*-propyl hydratropic alcohol
2691 Hexahydro-*para*-*iso*-propyl hydrocinnamic alcohol
1588 .... Hexahydro pseudoionone
2908 Hexahydro pyrethrone
2626 Hexahydro pyridine
1589 .... Hexahydro tetramethyl naphthalenone (isomerides)
1841 Hexahydro thymol
1976 Hexahydro-*ortho*-tolylacetate
1977 Hexahydro-*para*-tolylacetate
1577 Hexakose
1590 .... *gamma*-Hexalactone
1592 Hexaldehyde
1593 Hexaldehyde diethyl acetal
1594 Hexaldehyde dimethyl acetal
986 Hexaldehyde-*2,2*-dimethyl-*1,3*-propanediol (cyclic) acetal
776 Hexalin
86 "Hexalon"
1591 .... Hexamethylene carboxylate
2862 *2,6,10,15,19,23*-Hexamethyl-*2,6,10,14,18,22*-tetracosahexaene
1592 .... *n*-Hexanal
1593 .... Hexanal diethyl acetal
1594 .... Hexanal dimethyl acetal
2040 Hexane-*2*-carboxylic acid
54 Hexane dioic acid
31 *2,3*-Hexane dione
22 *2,5*-Hexane dione
1084 *3,4*-Hexane dione
1834 *1,2,3,4,5,6*-Hexane hexol (Mannitol)
2860 *1,2,3,4,5,6*-Hexane hexol (Sorbitol)
1595 "Hexane methyl benzyl thional"
1595 .... Hexane methylthional
1595 *1*-Hexane thiol (see also 1673)
1596 .... Hexanoic acid
1597 .... Hexanol
1925 *iso*-Hexanol
1590 Hexanolide-*1:4*
1933 *iso*-Hexanone-*2*
2404 Hexanoyl ethanol
1636 Hexanyl ethanoate
2626 Hexazane
1598 .... *cis-3*-hexenal
1599 .... *trans-2*-hexenal
2015 "*iso*-Hexenal"
1600 .... *trans-2*-Hexenal diethyl acetal
1601 .... *cis-3*-Hexenal-di-*cis-3*-hexenyl acetal
1602 .... *trans-2*-Hexenal-di-*cis-3*-hexenyl acetal
1603 Hexen-*2*-oic acid
1603 .... *trans-2*-Hexenoic acid
1603 *alpha-beta*-Hexenoic acid
1606 *alpha-beta*-Hexenol
1604 .... *cis-3*-Hexenol
1605 .... *iso*-Hexenol
1604 *n-beta*-Hexenol
1604 *beta-gamma*-Hexenol
1605 "*iso-beta-gamma*-Hexenol" (see also 1607)
1606 .... *trans-2*-Hexenol
1607 .... *trans-3*-Hexenol
2054 *omega*-Hexenol methylether
1609 *2*-Hexenyl acetate
1608 .... *cis-3*-Hexenyl acetate
1608 *cis-beta-gamma*-Hexenyl acetate
1609 .... *trans-2*-Hexenyl acetate
1610 .... *iso*-Hexenyl acetate
1610 "*iso-beta-gamma*-Hexenyl acetate"
1746 *secondary*-Hexenyl acetate
2358 "Hexenyl acetone"
1611 .... *cis-3*-Hexenyl anthranilate
1612 .... *cis-3*-Hexenyl benzoate
1619 *beta-gamma*-Hexenyl-*trans-2*-butenoate
1615 *2*-Hexenyl-*n*-butyrate
1613 .... *cis-3*-Hexenyl butyrate
1614 .... *cis-3*-Hexenyl-*iso*-butyrate
1613 *beta-gamma*-Hexenyl-*n*-butyrate
1614 *beta-gamma*-Hexenyl-*iso*-butyrate
1615 .... *trans-2*-Hexenyl butyrate
845 *gamma-3*-Hexenyl butyrolactone
1616 .... *cis-3*-Hexenyl caproate
1617 .... *trans-2*-Hexenyl caproate
1618 .... *cis-3*-Hexenyl cinnamate
1619 .... *cis-3*-Hexenyl crotonate
2162 *iso*-Hexenyl cyclohexene carboxaldehyde
920 *cis-3*-Hexenylether
1620 .... *cis-3*-Hexenyl formate
1617 *2*-Hexenyl-*n*-hexanoate
1616 *beta-gamma*-Hexenyl hexoate
1621 .... Hexenylidene methylanthranilate
1620 *beta-gamma*-Hexenyl methanoate
1622 *cis-3*-Hexenyl-*2*-methylbutanoate
1632 *beta-gamma*-Hexenyl-*3*-methylbutanoate
1630 *cis-3*-Hexenyl-*2*-methyl-*trans-2*-butenoate
1631 *trans-2*-Hexenyl-*2*-methyl-*trans-2*-butenoate
1622 .... *cis-3*-Hexenyl-*alpha*-methyl butyrate
1633 *trans-2*-Hexenyl-*3*-methylbutyrate
2078 *alpha*-Hexenyl-*gamma*-methyl butyrolactone
2054 *1*-Hexen-*6*-yl methylether
1298 *iso*-Hexenyl methylglycidic acid, ethylether
1627 *cis-3*-Hexen-*1*-yl-*2*-oxopropanoate
1632 *beta-gamma*-Hexenyl-*iso*-pentanoate

1623 .... *cis-3*-Hexenyl phenylacetate
1624 .... *trans-2*-Hexenyl phenylacetate
1618 *beta-gamma*-Hexenyl phenylacrylate
1626 *2*-Hexenyl propanoate
1625 *beta-gamma*-Hexenyl propanoate
1625 .... *cis-3*-Hexenyl propionate
1626 .... *trans-2*-Hexenyl propionate
1627 .... *cis-3*-Hexen-*1*-yl pyruvate
1628 .... *cis-3*-Hexenyl salicylate
1628 *beta-gamma*-Hexenyl salicylate
2162 *iso*-Hexenyl tetrahydrobenzaldehyde
1629 .... *cis-3*-Hexenyl-tetrahydro-*2*-pyranylether
1630 .... *cis-3*-Hexenyl tiglate
1631 .... *trans-2*-Hexenyl tiglate
1623 *beta-gamma*-Hexenyl-*alpha*-toluate
1632 .... *cis-3*-Hexenyl-*iso*-valerate
1633 .... *trans-2*-Hexenyl valerate
1633 *trans-2*-Hexenyl-*n*-valerate
1633 *trans-2*-Hexenyl-*iso*-valerate
2078 Hexenyl-*gamma*-valerolactone
2635 Hexitans
1596 *n*-Hexoic acid
1592 Hexoic aldehyde
1464 Hexose
1634 .... *2*-Hexoxyacetaldehyde dimethyl acetal
1635 .... *2*-Hexoxyacetaldehyde di-propylene-glycol hemi-acetal
1636 .... Hexyl acetate
1637 .... *iso*-Hexyl acetate (see also 1900)
1264 Hexyl acetoacetic ester
1638 .... *2*-Hexyl-*4*-(or-*5*-)-acetoxy tetrahydrofuran
2439 *alpha-n*-Hexylacetylene
2356 *3*-Hexyl acrolein
2356 *beta*-Hexyl acrolein
1597 *n*-Hexyl alcohol
2157 *active*-Hexyl alcohol
1592 Hexyl aldehyde
1639 .... *n*-Hexyl angelate
1640 .... Hexyl anisate
1641 .... Hexyl anthranilate
1642 .... Hexyl benzoate
1643 .... *n*-Hexyl benzoyl acetate
1644 .... Hexyl benzyl ether
1645 *n*-Hexyl-*n*-butanoate
1646 *n*-Hexyl-*iso*-butanoate
1647 *iso*-Hexyl-*n*-butanoate
467 Hexyl-*n*-butyl ketone
1645 .... Hexyl butyrate
1646 .... Hexyl-*iso*-butyrate
1647 .... *iso*-Hexyl-*n*-butyrate
1648 .... *alpha*-Hexyl-*gamma*-butyrolactone
1649 .... *alpha-iso*-Hexyl-*gamma-n*-butyrolactone
828 *gamma-n*-Hexyl-*gamma*-butyrolactone
1650 .... Hexyl caproate
1651 .... Hexyl caprylate
1501 Hexyl carbinol
1653 *alpha-n*-Hexyl cinnamal
1652 .... Hexyl cinnamate
1653 .... Hexyl cinnamic aldehyde
1657 Hexyl cyclohexane butyrate
1654 .... *n*-Hexyl-*4*-cyclohexanone
1655 .... *iso*-Hexyl-*2*-cyclohexanone
1656 .... *iso*-Hexyl-*4*-cyclohexanone
1655 *ortho-iso*-Hexyl cyclohexanone
1656 *para*-Hexyl cyclohexanone
1656 *para-iso*-Hexyl cyclohexanone
1657 .... Hexyl cyclohexyl butyrate
1658 .... *2*-Hexyl cyclopentanone
1658 *alpha-n*-Hexyl cyclopentanone
955 *n*-Hexyl cyclopentenone
1659 .... *2-n*-Hexyl-*2*-cyclopenten-*1*-one
2068 Hexyl-*3,3*-dimethylacrylate
1639 *n*-Hexyl-*cis-2,3*-dimethylacrylate
1682 *n*-Hexyl-*trans-alpha-beta*-dimethylacrylate
1660 .... *2*-Hexyl-*1,3*-dioxolane
1672 *n*-Hexyl dodecanoate
1672 *n*-Hexyl dodecylate
2156 Hexylene glycol
2346 Hexylene glycol diacetate
1603 *alpha-beta*-Hexylenic acid
1599 *alpha-beta*-Hexylenic aldehyde
1598 *beta-gamma*-Hexylenic aldehyde
1661 .... Hexyl ethyl carbonate
1926 *iso*-Hexyl ethylether
2351 Hexyl ethyl ketone
1662 .... Hexyl-*iso*-eugenol
1663 .... Hexyl formate
921 Hexyl fumarate
1664 Hexyl furan-*alpha*-carboxylate
1664 .... *n*-Hexyl furoate
1664 Hexyl-*2*-furoate
1665 .... *secondary*-Hexyl furoate
1666 .... *alpha*-Hexyl furfuracrolein
1666 *alpha-n*-Hexyl-*beta-2*-furylacrolein
1667 *n*-Hexyl heptanoate
1667 .... Hexyl heptoate
1667 Hexyl heptylate
1668 .... *n*-Hexyl-*n*-heptylether
1650 *n*-Hexyl hexanoate
1759 Hexyl hydracrylic aldehyde
1680 *n*-Hexyl-*ortho*-hydroxybenzoate
1498 *2*-Hexyl-*4*-hydroxy-*1,3*-dioxan
1671 Hexyl hydroxy ethoxyacetic caid, *delta*-lactone
1498 *2*-Hexyl-*4*-hydromethyl-*1,3*-dioxolan
1596 Hexylic acid
1669 .... *2-n*-Hexylidene cyclohexanone-*1*
1670 .... *alpha*-Hexylidene cyclopentanone
1670 *2-n*-Hexylidene cyclopentanone
1671 .... *2*-Hexyl-*5*-(or-*6*-)-keto-*1,4*-dioxane
1672 .... Hexyl laurate
2752 "*iso*-Hexyl levulinate"
1673 .... *n*-Hexyl mercaptan (see also 1595)
1681 *n*-Hexyl-*2*-mercapto ethanoate
1663 *n*-Hexyl methanoate
2068 Hexyl-*2*-methylbuten-*2*-oate-4
1639 *n*-Hexyl-*cis-2*-methyl-*2*-butenoate
1682 *n*-Hexyl-*trans-2*-methyl-*2*-butenoate
1674 .... Hexyl-*2*-methylbutyrate
2057 Hexyl methyl carbinol
2068 Hexyl-*beta*-methylcrotonate
1639 *n*-Hexyl-*cis-2*-methylcrotonate
2060 *para-iso*-Hexyl-*meta*-methyl cyclohexanol

1675 .... *2*-Hexyl-*5*-methyl-*1,3*-dioxolane
2065 *n*-Hexyl methylether
2066 *n*-Hexyl methyl ketone
1676 *n*-Hexyl nonanoate
1676 *n*-Hexyl nonylate
1651 *n*-Hexyl octanoate
1651 *n*-Hexyl octoate
1651 *n*-Hexyl octylate
1676 .... Hexyl pelargonate
1684 *n*-Hexyl-*n*-pentanoate
1685 *n*-Hexyl-*iso*-pentanoate
1686 *iso*-Hexyl-*iso*-pentanoate
1677 .... Hexyl phenylacetate
1678 .... Hexyl phenylethyl carbinol
1679 *n*-Hexyl propanoate
2448 Hexyl propiolic aldehyde dimethyl acetal
1679 .... *n*-Hexyl propionate
2068 Hexyl-*iso*-propylidene acetate
1664 Hexyl pyromucate
1680 .... Hexyl salicylate
2068 Hexyl senecioate
1681 .... *n*-Hexyl thioglycolate
1682 .... Hexyl tiglate
1677 *n*-Hexyl-*alpha*-toluate
1683 *n*-Hexyl undecanoate
1683 .... Hexyl undecylate
1684 .... *n*-Hexyl-*n*-valerate
1685 .... *n*-Hexyl-*iso*-valerate
1686 .... *iso*-Hexyl-*iso*-valerate
3025 *alpha*-*n*-Hexyl-*delta*-valerolactone
1687 .... Hexyl vinyl carbinol
2359 Hexyl vinyl carbinyl acetate
2810 Hiba oil (Japanese)
2445 "Hibiscolide"
2206 Hinoki leaf oil (see also 2207)
1751 "H.M.F."
1134 "Homo-*ortho*-acetanisole"
1068 "Homo ambrettemusk"
1092 "Homo ambriol"
1688 .... Homo anethole
1135 "Homo anisaldehyde" (see also 1882)
1886 "Homo anisylacetone"
1689 .... Homocatechol dimethylether
1873 Homocatechol methyl ethylether
705 Homocatechol nomomethyl ether
1690 .... Homocetyl alcohol
1691 .... Homocinnamyl alcohol
1190 "Homo citral"
1192 "Homo citronellol"
980 Homo coniferaldehyde
1251 "Homo creosol"
751 "Homo cuminic acid"
2739 "Homo cuminic alcohol"
2734 "Homo cuminic aldehyde"
495 "Homo cyclamenaldehyde"
2704 "Homo dihydroeugenol"
2064 "Homo dihydrojasmone"
2049 "Homo dihydro-*iso*-jasmone"
2016 "Homo-D.M.B.C."
2017 "Homo-D.M.B.C.A."
2168 "Homo-dulcin"
1890 "Homo ethone"
771 "Homo exaltone"
1246 "Homo geraniol"
1248 "Homo geranylacetone"
1136 "Home guaiacol"
1692 .... Homo heliotropine
1535 "Homo-*iso*-jasmone"
1279 "Homo linalool"
1280 "Homo linalylacetate"
1281 "Homo linalylacetate epoxide"
1693 .... Homo menthylsalicylate
1687 "Homo mitsutake-alcohol"
1068 "Homo musk ambrette"
2114 "Homo myrac aldehyde"
1314 "Homo neofolione"
165 "Homo patchone"
1346 *4*-Homopicoline
1346 *gamma*-Homopicoline
1174 Homopinacone
1692 Homopiperonal
1692 Homo protocatechualdehyde methylene ether
1694 .... Homoquinoline
2240 "Homo safranal"
1273 "Homo skatole"
2856 "Homo sodium cyclamate"
1331 "Homo syringa aldehyde"
2015 "Homo tiglic aldehyde"
1695 .... Homovanillin
2649 "Homo vanitrope"
1365 Homo veratraldehyde (see also 2069)
1689 Homo veratrole
584 Humulene
1696 Hyacinthal
2470 "Hyacinth aldehyde"
371 "Hyacinthin" (see also 2470)
2485 "Hyacylene"
1728 Hycelea
1762 Hydracrylic aldehyde-*iso*-amylether
1763 Hydracrylic aldehyde benzylether
1696 .... Hydratropaldehyde
1697 .... Hydratropaldehyde dibenzylacetal
1698 .... Hydratropaldehyde di-*iso*-butylacetal
1699 .... Hydratropaldehyde diethylacetal
1700 .... Hydratropaldehyde dimethylacetal
1701 .... Hydratropaldehyde-*2,4*-dioxy-*4*-methylpentane acetal
1702 .... Hydratropaldehyde di-phenylethyl acetal
1703 .... Hydratropaldehyde ethyleneglycol acetal
1704 .... Hydratropaldehyde propyleneglycol acetal
2578 Hydratropic acid
1707 Hydratropic alcohol
1696 Hydratropic aldehyde
1705 .... Hydratropyl acetate
1706 .... Hydratropyl acetone
1707 .... Hydratropyl alcohol
1708 .... Hydratropyl butyrate
1709 .... Hydratropyl-*iso*-butyrate
1715 Hydrindole
1710 .... *alpha*-Hydrindone
1711 .... *beta*-Hydrindone
2 Hydroabietyl alcohol
1712 .... Hydrocardanol
2580 Hydrocinnamaldehyde
2579 Hydrocinnamic acid

2589 Hydrocinnamic alcohol
2580 Hydrocinnamic aldehyde
2581 Hydrocinnamic aldehyde diethyl acetal
2582 Hydrocinnamic aldehyde-*2,4*-dihydroxy-*4*-methylpentane acetal
2583 Hydrocinnamic aldehyde dimethyl acetal
2584 Hydrocinnamic aldehyde di-phenylethyl acetal
2585 Hydrocinnamic aldehyde ethylene-glycol (cyclic) acetal
2586 Hydrocinnamic nitrile
2588 Hydrocinnamyl acetate
2589 Hydrocinnamyl alcohol
2590 Hydrocinnamyl benzoate
2591 Hydrocinnamyl-*n*-butyrate
2592 Hydrocinnamyl-*iso*-butyrate
2596 Hydrocinnamyl cinnamate
2597 Hydrocinnamyl cyanide
2593 Hydrocinnamyl decylate
2598 Hydrocinnamyl formate
2594 Hydrocinnamyl hexanoate
2203 Hydrocinnamyl methylether
2595 Hydrocinnamyl octoate
2599 Hydrocinnamyl phenylacetate
2600 Hydrocinnamyl propionate
2601 *2*-Hydrocinnamyl pyridine
2601 *4*-Hydrocinnamyl pyridine
2602 *2*-Hydrocinnamyl tetrahydrofuran
2599 Hydrocinnamyl-*alpha*-toluate
2603 Hydrocinnamyl undecenoate
2604 Hydrocinnamyl-*n*-valerate
2605 Hydrocinnamyl-*iso*-valerianate
934 Hydrocoumarin
936 Hydrocumin alcohol
937 Hydrocuminic aldehyde
1713 .... Hydrocyanic acid
1714 .... Hydrogen sulfide
1715 .... Hydroindol
962 *delta*-Hydromethyl ionone
1716 .... Hydroquinaldine
1717 Hydroquinol
1717 .... Hydroquinone
1718 .... Hydroquinone diethyl ether
1719 .... Hydroquinone dimethyl ether
1720 .... Hydroquinone methyl ethyl ether
1861 Hydroquinone methyl methallyl ether
1721 .... Hydroquinone monoethyl ether
1722 .... Hydroquinone monomethyl ether
469 Hydroquinone monomethyl ether, butylated
1714 "Hydrosulfuric acid"
2942 Hydro thymoquinone
1429 *beta*-Hydroxyacetaldehyde diethyl acetal, geranylether
1634 *beta*-Hydroxyacetaldehyde dimethyl acetal, hexylether
2430 *beta*-Hydroxyacetaldehyde, octylether
1429 *beta*-Hydroxyacetal geranylether
34 Hydroxyacetone
1723 .... *ortho*-Hydroxy acetophenone
1724 .... *para*-Hydroxy acetophenone
1723 *2*-Hydroxyacetyl benzene
1724 *4*-Hydroxyacetyl benzene
2077 *4*-Hydroxy-*5*-acetyltoluene
2844 *beta*-Hydroxy alanine
606 *1*-Hydroxy-*4*-allylbenzol
2839 *2*-(*alpha*-Hydroxyamyl)-cyclohex-*2*-ene-*1*-carboxylic acid
2840 *2*-(*alpha*-Hydroxyamyl)-cyclohex-*2*-ene-*1*-carboxylic acid, lactone
1889 *2*-Hydroxy anisaldehyde
1472 *ortho*-Hydroxy anisole
1722 *para*-Hydroxy anisole
1725 .... *para*-Hydroxy benzalacetone
2815 *ortho*-Hydroxy benzaldehyde
1726 .... *para*-Hydroxy benzaldehyde
241 *para*-Hydroxybenzaldehyde methyl-ether
1760 *para*-Hydroxy benzylacetone
1095 *ortho*-Hydroxy benzylalcohol-di-*iso*-propylketal
2488 *5*-Hydroxy-*2*-benzyl-*1,3*-dioxan
1725 *para*-Hydroxy benzylidene acetone
899 *beta*-Hydroxy-*beta*-benzylpentane
989 *beta*-Hydroxy-*beta*-benzylpropane
350 *2*-Hydroxybornane
391 *2*-Hydroxybutane
1271 *2*-Hydroxybutane-*2*-carboxylic acid, ethylester
1829 *l*-Hydroxybutane dioic acid
43 *3*-Hydroxy-*2*-butanone
504 *1*-Hydroxy-*4*-*tertiary*-butylbenzene
469 *1*-Hydroxy-*2*-(and-*3*-)-*tertiary*-butyl-*4*-methoxybenzene
522 *3*-(or-*4*-)-Hydroxybutyric acid, lactone
350 *2*-Hydroxy camphane
1727 *gamma*-Hydroxy-*n*-caproaldehyde
1727 .... *gamma*-Hydroxy caproic aldehyde
704 *ortho*-Hydroxycinnamic acid, lactone
1728 .... Hydroxycitronellal
1729 .... Hydroxycitronellal di-*iso*-butyl acetal
1730 .... Hydroxycitronellal diethyl acetal
1731 .... Hydroxycitronellal dimethyl acetal
1732 .... Hydroxycitronellal di-phenylethyl acetal
1733 .... Hydroxycitronellal ethylanthranilate
1734 .... Hydroxycitronellal linalylanthranilate
1735 .... Hydroxycitronellal methylanthranilate
1870 Hydroxycitronellal methylether
1736 .... Hydroxycitronellidene-*para*-tolyl methyl ketone
1737 .... Hydroxycitronellol
1738 .... Hydroxycitronellyl ethylcarbonate
1739 .... *4*-Hydroxy coumarin
3020 *7*-Hydroxy coumarin
2733 *para*-Hydroxy cumene
37 *1*-Hydroxy cyclohexyl methyl ketone
573 *2*-Hydroxy-*para*-cymene
2944 *3*-Hydroxy-*para*-cymene
1740 .... *1*-Hydroxy-*3*-decanone
934 *ortho*-Hydroxy-dihydrocinnamic acid, lactone
1737 Hydroxy dihydrocitronellol
1741 .... *2*-Hydroxy-*4,6*-dimethoxy acetophenone

1742 .... *4*-Hydroxy-*3,5*-dimethoxy benzaldehyde
3098 *2*-Hydroxy-*1,3*-dimethylbenzene
3098 *2*-Hydroxy-*1,4*-dimethylbenzene
3098 *3*-Hydroxy-*1,2*-dimethylbenzene
3098 *4*-Hydroxy-*1,2*-dimethylbenzene
3098 *4*-Hydroxy-*1,3*-dimethylbenzene
3098 *5*-Hydroxy-*1,3*-dimethylbenzene
1743 .... *2*-Hydroxy-*4,4*-dimethyl-*4*-cyclohexyl butane
1804 *2*-Hydroxy-*2,6*-dimethyl-*3,6*-epoxyocten-*7*
1025 *4*-Hydroxy-*2,5*-dimethyl-*3(2H)*-furanone
1728 *7*-Hydroxy-*3,7*-dimethyloctan-*1*-al
2199 *2*-Hydroxy-*4,4'*-dimethyl-*4*-phenylbutane
1103 *5*-Hydroxydodecanoic acid, *delta*-lactone
1364 *3*-Hydroxy-*4*-ethoxybenzaldehyde
2704 *3*-Hydroxy-*4*-ethoxy propylbenzene
1874 *ortho*-Hydroxyethylanisate
1328 *2*-Hydroxy ethylbenzene
1329 *4*-Hydroxy ethylbenzene
2513 *beta*-Hydroxy ethylbenzene
1350 *2*-Hydroxy ethylbenzoate
1744 .... *2*-Hydroxyethyl-*2*-bornanylether
1201 *1*-Hydroxy-*4*-ethylcyclohexane
2906 *alpha*-*2*-Hydroxyethylfuran
1132 *2*-*alpha*-Hydroxyethyl hexahydropyridine
2243 *5*-*beta*-Hydroxyethyl-*4*-methyl-thiazole
1223 *beta*-Hydroxyethyl phenylether
1745 .... *3*-Hydroxy-*2*-ethyl-*4*-pyrone
2012 *beta*-Hydroxy ethylsalicylate
703 *gamma*-Hydroxy-*iso*-eugenol
1832 *3*-Hydroxy-*2*-furylmethylketone
1501 *1*-Hydroxyheptane
1502 *2*-Hydroxyheptane
1503 *3*-Hydroxyheptane
1904 *2*-Hydroxy-*6*-heptene
923 *16*-Hydroxyhexadecanoic acid, lactone
105 *16*-Hydroxy-Δ*7*-hexadecenoic acid, lactone
1577 *1*-Hydroxy-*2,4*-hexadiene
1727 *gamma*-Hydroxy-*n*-hexanal
2079 *beta*-Hydroxyhexanoic acid, methylester
1746 .... *4*-Hydroxy-*2*-hexenylacetate
1832 *5*-Hydroxy-*2*-hydroxymethyl-*gamma*-pyrone
1715 *1*-Hydroxyindane
1747 *2*-Hydroxy-*4*-methoxyacetone
28 *1*-Hydroxy-*2*-methoxy acetophenone
1747 .... *2*-Hydroxy-*4*-methoxy acetophenone
1748 .... *2*-Hydroxy-*5*-methoxy acetophenone
28 *1*-Hydroxy-*2*-methoxy-*4*-acetylbenzene
3101 *4*-Hydroxy-*3*-methoxy benzalacetone
1888 *2*-Hydroxy-*3*-methoxybenzaldehyde
1889 *2*-Hydroxy-*4*-methoxybenzaldehyde
3068 *3*-Hydroxy-*4*-methoxybenzaldehyde
3067 *4*-Hydroxy-*3*-methoxybenzaldehyde
3066 *4*-Hydroxy-*3*-methoxy benzoic acid
1879 *2*-Hydroxy-*4*-methoxybenzoic acid, methylester
3073 *4*-Hydroxy-*3*-methoxy benzylalcohol
2353 *N*-(*4*-Hydroxy-*3*-methoxybenzyl)-nonanamide
703 *4*-Hydroxy-*3*-methoxycinnamic alcohol
702 *4*-Hydroxy-*3*-methoxycinnamic alcohol
1251 *1*-Hydroxy-*2*-methoxy-*4*-ethylbenzene
1874 *2*-Hydroxy-*4*-methoxy ethylbenzoate
451 *6*-Hydroxy-*4*-methoxy-*2*-methyl-benzoic acid, *iso*-butylester
1234 *2*-Hydroxy-*4*-methoxy-*6*-methyl-benzoic acid, ethylester
2028 *6*-Hydroxy-*4*-methoxy-*2*-methyl-benzoic acid, methylester
705 *1*-Hydroxy-*2*-methoxy-*4*-methylbenzol
1695 *4*-Hydroxy-*3*-methoxy phenylacetaldehyde
3074 *4*-(*4'*-Hydroxy-*3*-methoxyphenyl)-*3*-buten-*3*-one
2845 *1*-(*4*-Hydroxy-*3*-methoxyphenyl)-*4*-decen-*3*-one
3101 (*4*-Hydroxy-*3*-methoxyphenyl)-methyl ketone
2845 (*4*-Hydroxy-*3*-methoxyphenyl)-ethyl-*n*-*alpha*-*beta*-heptenyl ketone
703 *3*-(*4*-Hydroxy-*3*-methoxyphenyl)-*2*-propen-*1*-ol
3094 *3*-Hydroxy-*4*-methoxy styrene
1891 *4*-Hydroxy-*3*-methoxy styrene
2442 *3*-Hydroxy-*5*-methoxy toluene
451 *6*-Hydroxy-*4*-methoxy-*ortho*-toluic acid, *iso*-butylester
2028 *6*-Hydroxy-*4*-methoxy-*ortho*-toluic acid, methylester
2081 *2*-Hydroxy-*3*-methylacetophenone
1749 .... *1*-Hydroxy-*2*-methyl-*4*-*tertiary*-amylcyclohexane
2646 Hydroxy methylanethole
1879 *ortho*-Hydroxy methylanisate
2488 *5*-Hydroxymethyl-*2*-benzyl-*1,3*-dioxolan
942 *2*-Hydroxymethyl bicyclo (*2:2:1*)-heptane
1750 .... *gamma*-Hydroxy-*gamma*-methyl-*n*-caproic aldehyde
1987 *2*-Hydroxy-*3*-methyl-*2*-cyclopenten-*1*-one
1751 *5*-(Hydroxymethyl)-*2*-formylfuran
1751 .... *5*-(Hydroxymethyl)-*2*-furaldehyde
1416 *2*-Hydroxymethyl furan
1751 *5*-(Hydroxymethyl)-*2*-furancarbonal
1751 *5*-(Hydroxymethyl)-*2*-furfural
1751 Hydroxymethyl furfural
1750 *3*-Hydroxy-*3*-methyl hexanal
2060 *2*-Hydroxy-*4*-methyl-*1*-hexyl cyclohexane
2060 *4*-Hydroxy-*6*-methyl-*1*-*iso*-hexyl cyclohexane
1752 .... *3*-Hydroxymethyl-*2*-nonanone
1753 .... *3*-Hydroxymethyl-*2*-octanone

1754 .... *4*-(*4*-Hydroxy-*4*-methyl pentyl)-*3*-cyclohexene-*10*-carboxaldehyde
273 *4*-Hydroxymethyl-*2*-phenyl-*meta*-dioxolane
390 *1*-Hydroxymethyl propane
936 *1*-Hydroxymethyl-*4*-*iso*-propenyl-*1*-cyclohexene
1831 *3*-Hydroxy-*2*-methyl-(*1*,*4*-pyran)
1831 *3*-Hydroxy-*2*-methyl-*gamma*-pyrone
1832 *5*-Hydroxy-*2*-methyl-*gamma*-pyrone
1948 *2*-Hydroxy-*4*-methylquinoline
1755 .... *14*-Hydroxy-*13*-methyl-*1*-tetradecanoic acid, lactone
2335 *1*-Hydroxy-*4*-nitrobenzene
1759 *beta*-Hydroxynonanal
2350 *4*-Hydroxynonanoic acid, lactone
1756 .... *1*-Hydroxy-*3*-nonanone (see also 1753)
1757 .... *5*-Hydroxy-*4*-octanone
2445 *16*-Hydroxy-*12*-oxahexadecanoic acid, *omega*-lactone
43 *gamma*-Hydroxy-*beta*-oxybutane
1758 .... *14*-Hydroxy-*4*-oxy-Tetradecyl lactone
1759 .... *beta*-Hydroxy pelargonic aldehyde
811 *15*-Hydroxypentadecanoic acid, lactone
812 Hydroxypentadecanone
1136 *ortho*-Hydroxyphenethol
1721 *para*-Hydroxyphenethol
277 *2*-Hydroxy-*2*-phenylacetophenone
1760 .... *para*-Hydroxy phenylbutanone
1725 *para*-Hydroxy phenylbutenone
273 *5*-Hydroxy-*2*-phenyl-*1*,*3*-dioxane
1761 *beta*-*para*-Hydroxy phenylethanol
1761 .... *para*-Hydroxy phenylethyl alcohol
1760 *para*-Hydroxy phenylethyl methyl ketone
2432 *4*-(*para*-Hydroxyphenyl)-*2* : *2* : *4* : *4*-tetramethylbutane
1069 *2*-Hydroxypiperitone
657 *2*-Hydroxy-*1*,*2*,*3*-propanetricarboxylic acid
2650 *4*-Hydroxy-*1*-*para*-propenylbenzene
1792 *alpha*-Hydroxypropionic acid
1792 *2*-Hydroxypropionic acid
1762 .... *beta*-Hydroxypropionic aldehyde-*iso*-Amylether
1763 .... *beta*-Hydroxypropionic aldehyde benzylether
1764 .... *beta*-Hydroxypropionic aldehyde diethyl acetal, *iso*-amylether
1765 .... *beta*-Hydroxypropionic aldehyde diethyl acetal, benzylether
1766 .... *beta*-Hydroxypropionic aldehyde diethyl acetal, phenylether
1767 .... *beta*-Hydroxypropionic aldehyde diethyl acetal, -*meta*-(and *ortho*-) tolylether
2718 *para*-Hydroxy propylbenzoate
485 *2*-Hydroxy-*iso*-propyl-*5*-*iso*-butyl-*5*-vinyl tetrahydrofuran
1768 .... *2*-Hydroxypropyl-*para*-*N*,*N*-*bis*(*2*-hydroxypropyl)-aminobenzoate
2245 *gamma*-Hydroxypropyl methylsulfide
1804 *2*-Hydroxy-*iso*-propyl-*5*-methyl-*5*-vinyl tetrahydrofuran
1224 *beta*-Hydroxypropyl phenylether
1829 *2*-Hydroxysuccinic acid
290 *alpha*-Hydroxytoluene
707 *3*-Hydroxytoluene
708 *4*-Hydroxytoluene
1833 *alpha*-Hydroxy-*alpha*-toluic nitrile
2966 *2*-Hydroxy-*4*(*para*-tolyl)-butane
657 *beta*-Hydroxy tricarballylic acid
1769 .... *delta*-Hydroxy valeric aldehyde
1728 "Hylea"
24 Hypnone
2346 "Hyxis"

# I

1770 .... Ianthone
1771 .... Ibotenic acid
2783 Imidole
471 "Improvol"
1715 Indan-*1*-ol
1710 *1*-Indanone
1711 *2*-Indanone
1772 .... Indole
1773 .... Indolene
1774 .... Indole-phenylacetaldehyde
1773 *8*,*8*-*bis*-(*3H*-Indol-*3*-yl)-*2*,*6*-dimethyl-*2*-octanol
1774 *beta*-*beta*-*bis*-(*3H*-Indol-*3*-yl)-*alpha*-phenylethylene
3036 "Intreleven aldehyde"
471 "Ionol"
1775 .... *beta*-Ionol
1776 .... Ionones, summary
1777 .... *alpha*-Ionone
1778 .... *beta*-Ionone
1779 .... *gamma*-Ionone
1780 .... *beta*-Ionone epoxide
1781 .... *alpha*-Ionone ethylglycidate
1782 .... *alpha*-Ionone methylanthranilate
1783 .... *alpha*-Ionone methylglycidate
2661 I.P.A.
510 "Iphaneine"
2087 "Iraldeine beta"
2086 "Iraldeine gamma"
2088 "Iraldeine delta"
166 "Irinone"
2356 "Iris aldehyde"
3002 "Iritone"
2088 "Ironal methyl delta"
1784 .... *alpha*-Irone*)
*) A summary of Neo-irones is given in monograph No.2312.
1785 .... *beta*-Irone
1786 .... *gamma*-Irone
530 "Isonefolia"

# J

2485 "Jacinthal"
565 Japan camphor
2346 Jasmal (see also 1409)
157 "Jasmalique"
826 "Jasmalol"
288 "Jasmarol"
2346 "Jasmelia"
149 Jasmin aldehyde
1787 .... Jasmine lactone

1653 Jasminolene
710 "Jasmin oxide"
149 Jasminyl
149 Jasmonal (see also 1654)
1653 Jasmonal H
1788 .... *cis*-Jasmone
1789 .... "*iso*-Jasmone"
954 *iso*-Jasmone (see also 1659 and 1670)*)
2077 "*iso*-Jasmone de Darzens"
1790 .... *trans*-Jasmone
1787 Jasmone lactone
2346 Jasmonyl
149 Jasmylal
2346 "Jessemal"

**K**
2860 "Karion"
1800 Kautschin
2192 Keora oil
1055 Ketine
13 Ketobepine
1798 *3*-Ketobutane-*1*-carboxylic acid
814 Ketocyclopentane
777 Ketohexamethylene
1710 *1*-Ketoindane
1711 *2*-Ketoindane
1987 Ketonarome
2404 "Ketone alcohol"
2352 "Ketone alcohol ester"
1791 .... Ketone BD-9
2020 Ketone C-4
1905 Ketone C-7
2279 Ketonmoskus
814 Ketopentamethylene
18 Ketopropane
2785 *alpha*-Ketopropionic acid
2786 *alpha*-Ketopropionic aldehyde
2786 *1,2*-Ketopropionic aldehyde
266 *L-3*-Ketothreohexuronic acid, lactone
565 *2*-Keto-*1*,*7*,*7*-trimethyl norcamphane
1798 *gamma*-Ketovaleric acid
483 *gamma*-Ketovaleric acid, *n*-butylester
2192 Kewda oil
1832 Kojic acid
2980 Kronitex

**L**
424 "Labdanol"
1792 .... Lactic acid
417 Lactic acid, butylester, butyrate
1182 Lactic acid, ethylester, butyrate
1793 Lactobiose
1793 .... Lactose
1793 *alpha*-Lactose monohydrate
1798 Laevulic acid
1831 Laricin
1831 Larixinic acid
1223 "Larosol"
3021 Laurel (California laurel)
1113 Lauric acetate
1107 Lauric acid
1108 Lauric alcohol
1105 Lauric aldehyde
1106 Lauric aldehyde dimethylacetal
1728 "Laurinal"
1728 "Laurine"
1107 Laurostearic acid
1113 Lauryl acetate
1108 Lauryl alcohol
2258 *iso*-Lauryl alcohol
1105 Lauryl aldehyde
1114 Lauryl benzoate
1115 Lauryl butyrate
1116 Lauryl-*iso*-butyrate
1119 Lauryl formate
1537 Lauryl heptyl ether
1537 Lauryl heptyl oxide
1120 Lauryl mercaptan
1123 Lauryl pentanoate
1122 Lauryl propionate
1124 Lauryl-*iso*-valerate
789 "Lavamenthe"
2909 "Lavandor"
2910 "Lavandor acetate"
2911 "Lavandor butyrate"
2912 "Lavandor-*iso*-butyrate"
2171 "Lavandozon"
1794 .... Lavandulol
1795 .... Lavandulyl acetate
1796 .... *dl*-Lavandulyl-*alpha*-methylbutyrate
7 Leaf acetal (see also 10)
1604 Leaf alcohol (see also 1606)
7 Leaf alcohol acetal
1598 Leaf aldehyde (see also 1599)
1797 .... Ledol
1797 "Ledum camphor"
649 "Lemarome"
2235 Lepidine
1948 *2*-(*1*)-Lepidine
2791 Leucoline
670 "Levocitrol"
1798 .... Levulinic acid
1803 "Licareol"
2028 "Lichenol" (see also 2747)
997 "Lichenone"
1471 Licorice
3081 Lignolia
2384 "Lignyl acetate"
475 Ligusticum lactone
925 "Ligustilide"
2236 "Lilacine"
1700 "Lilanthal"
496 "Lilial"
1799 .... Lilial-methylanthranilate
759 "Lilianthol" (see also 1799)
1728 "Lily aldehyde" (see also 496)
758 "Lime aldehyde"
1800 .... *d*-Limonene
1074 *dl*-Limonene
1801 .... *l*-Limonene
1074 *racemic*-Limonene
1802 .... Limonene diol
1802 Limonene glycol
1803 .... Linalool
2097 Linalool methylether
1804 .... Linalool oxide
1805 .... Linalool oxide acetate

*) A summary of "Jasmone-type" materials is included in this work at the end of the monographs in volume II, immediately preceding the index.

1806 .... Linalyl acetate
1805 Linalyl acetate epoxide
1807 Linalyl-*ortho*-aminobenzoate
1807 .... Linalyl anthranilate
1808 .... Linalyl benzoate
1809 .... Linalyl butyrate
1810 .... Linalyl-*iso*-butyrate
1811 .... Linalyl caproate
1812 .... Linalyl caprylate
1813 .... Linalyl cinnamate
1814 .... Linalyl citronellate
1282 Linalyl ethylether
1815 .... Linalyl formate
1816 Linalyl heptanoate
1816 .... Linalyl heptoate
1816 Linalyl heptylate
1551 Linalyl heptylether
1811 Linalyl hexanoate
1811 Linalyl hexoate
1823 Linalyl-*ortho*-hydroxybenzoate
1817 Linalyl-*2*-methylaminobenzoate
1817 .... Linalyl-*N*-methylanthranilate
2097 Linalyl methylether
1818 Linalyl-*4*-methyl-*2*-pentenoate
1818 .... Linalyl methyltiglate
1819 Linalyl nonanoate
1819 Linalyl nonylate
1812 Linalyl octanoate
1812 Linalyl octoate
1822 Linalyl-*2*-oxopropanoate
1819 .... Linalyl pelargonate
1824 Linalyl-*n*-pentanoate
1825 Linalyl-*iso*-pentanoate
1820 .... Linalyl phenylacetate
1821 .... Linalyl propionate
1822 .... Linalyl pyruvate
1814 "Linalyl rhodinate"
1823 .... Linalyl salicylate
1820 Linalyl-*alpha*-toluate
1824 .... Linalyl-*n*-valerate
1825 .... Linalyl-*iso*-valerate
2980 Lindol
3067 "Lioxin"
2780 "Liquid smoke"
2315 "Lorena"
1108 "Lorol No. 5"
1108 "Lorol No. 9"
1108 "Lorol No. 11"
841 "Lorol No. 22"
1574 "Lorol No. 24"
2392 "Lorol No. 28"
703 Lubanol
1826 .... *alpha-alpha'*-Lutidine
1827 .... *alpha-gamma*-Lutidine
1827 *2*,*4*-Lutidine
1826 *2*,*6*-Lutidine
997 "Lychenone"
1754 "Lyral"
2080 "Lyral-methylanthranilate"

**M**

2013 "Madescol"
1480 "Madrysia"
2853 Magnesium cyclamate
149 "Mahonia"
1728 "Majal"
1828 .... Maleic acid
1411 *para*-Maleic acid
1829 .... *l*-Malic acid
1830 .... Malonic acid
910 Malonic ester
1831 .... Maltol
1832 .... *iso*-Maltol
2171 "Malvone" (see also 1193)
2365 "Mandarinol N.A."
1833 .... *dl*-Mandelonitrile
1834 Manna sugar
1834 Mannite
1834 .... Mannitol
1835 .... Manool
702 Maple aldehyde
1987 Maple lactone
2013 "Maraniol"
231 "Matsutake alcohol"
2020 M.E.K.
1895 "Melilone"
13 "Melilot"
1895 "Melilotal"
934 Melilotic acid, lactone
934 "Melilotine"
1895 "Melilot ketone"
13 "Melitone"
2513 "Mellol"
1831 "Mellotone"
1011 "Melonal"
1870 "Melonia"
2870 *meta*-Menthadiene-*1*,*8*(*9*)
2870 *meta*-Menthadiene-*6*,*8*(*9*)
937 *para*-Menthadien-*1*,*8*(*9*)-al-*7*
2873 *para*-Menthadiene-*1*,*3*
2874 *para*-Menthadiene-*1*,*4*
2882 *para*-Mentha-*1*,*4*(*8*)-diene
2459 *para*-Mentha-*1*,*5*-diene
2460 *1*(*7*),*2*-*para*-Menthadiene
1800 *d*-*para*-Mentha-*1*,*8*-diene
2882 *para*-Mentha-*2*,*4*(*8*)-diene
936 Menthadiene-*7*-carbinol
935 Menthadiene-*7*-carbinyl acetate
578 *laevo*-*para*-Mentha-*6*,*8*-dien-*2*-ol
936 *1*,*8*-*para*-Menthadien-*7*-ol
2629 *para*-Mentha-*1*,*8*(*9*)-dien-*3*-one
2628 *para*-Mentha-*1*,*4*(*8*)-dien-*3*-one
2861 *para*-Menthadien-*5*,*8*(*9*)-one-*2*
579 *6*,*8*-(or-*9*)-*para*-Menthadien-*2*-one
582 *l*-*para*-Mentha-*6*,*8*-dien-*2*-yl acetate
935 *1*,*8*-*para*-Menthadien-*7*-yl acetate
583 *l*-*para*-Mentha-*6*,*8*-dien-*2*-yl propionate
1836 .... *para*-Menthane
2880 *para*-Menthanediol-(*1*,*8*)-hydrate
1075 *para*-Menthane-*1*,*2*,*8*,*9*-tetrol
2313 *d*-*3*-*para*-Menthanol
1840 *l*-*3*-*para*-Menthanol
970 *para*-Menthan-*9*-ol
1843 *d*-(or-*l*)-*para*-Menthan-*3*-one
1844 *dl*-*cis*-*para*-Menthan-*3*-one
971 "Menthanyl acetate"
971 *para*-Menthan-*8*-yl acetate
2216 *3*-(*para*-Menthanyl)-butan-*2*-ol
2217 *3*-(*para*-Menthanyl)-butan-*2*-one
2915 *para*-Menthanyl carbinyl

tetrahydropyranyl ether
1837 .... Menthene
2458 *para*-Menthen-*7*-al
1802 *para*-Menthene-*8*(*9*)-diol-*1*,*2*
2625 *iso-1-para*-Menthene-*6*,*8*-diol
2876 *1-para*-Menthen-*4*-ol
2877 *para*-Menth-*1*-en-*8*-ol
2875 *Δ3-para*-Menthen-*1*-ol
2879 *Δ-4,8-para*-Menthenol-*1*
2767 *para*-Menthen-*4*-(*8*)-ol-*3*
926 *para*-Menth-*8*-(*9*)-en-*2*-ol
2768 *para*-Menth-*8*-en-*3*-ol
2878 *Δ-8,9-para*-Menthenol-*1*
1069 *1-para*-Menthen-*2*-ol-*3*-one
2630 *para*-Menth-*1*-en-*3*-one
2769 *para*-Menth-*4*-(*8*)-en-*3*-one
581 *para*-Menthen-*6*-one-*2*
2770 *para*-Menth-*8*-en-*3*-one
927 *cis-para*-Menthen-*8*-(*9*)-one-*2*
2883 *para*-Menth-*1*-en-*8*-yl acetate
928 *para*-Menth-*8*-(*9*)-en-*2*-yl acetate
2884 *para*-Menth-*1*-en-*8*-yl-*ortho*-aminobenzoate
2885 *para*-Menth-*1*-en-*8*-yl benzoate
2886 *para*-Menth-*1*-en-*8*-yl-*n*-butanoate
2887 *para*-Menth-*1*-en-*8*-yl-*iso*-butyrate
2888 *para*-Menth-*1*-en-*8*-yl cinnamate
2889 *para*-Menth-*1*-en-*8*-yl formate
2321 Menthenyl ketone
2893 *para*-Menth-*1*-en-*8*-yl-*beta*-methylbutyrate
2892 *para*-Menth-*1*-en--*8*yl pentanoate
2321 *1*-(*para*-Menthen-6-yl)-*1*-propanone
2891 *para*-Menth-*1*-en-*8*-yl propionate
2890 *para*-Menth-*1*-en-*8*-yl-*alpha*-toluate
1838 .... Menthofuran
1839 .... *dextro*-Menthol
1840 .... *laevo*-Menthol
1841 .... *dl*-Menthol
1842 .... *iso*-Menthol
1841 *racemic*-Menthol
1837 Menthomenthene
1836 Menthonaphthene
1843 .... Menthone
1844 .... *iso*-Menthone
1845 .... *laevo*-Menthyl acetate
1846 .... *dl*-Menthyl acetate
1845 *l-para*-Menth-*3*-yl acetate
1846 *racemic*-Menthyl acetate
1847 .... Menthyl anthranilate
1847 *para*-Menth-*3*-yl anthranilate
1848 .... Menthyl benzoate
1848 *para*-Menth-*3*-yl benzoate
1849 .... Menthyl-*iso*-butyrate
1849 *para*-Menth-*3*-yl-*iso*-butyrate
1693 Menthyl-*gamma*-cresotinate
1693 Menthyl-*meta*-cresotinate
1850 .... Menthyl formate
1850 *para*-Menth-*3*-yl formate
1693 Menthyl-*2*-hydroxy-*para*-toluate
1693 Menthyl-*4*-methylsalicylate
1851 .... *laevo*-Menthyl phenylacetate
1851 *para*-Menth-*3*-yl phenylacetate
1852 .... Menthyl propionate
1852 *para*-Menth-*3*-yl propionate
1853 .... Menthyl salicylate
1853 *para*-Menth-*3*-yl salicylate
1854 Menthyl valerate
1854 .... Menthyl-*iso*-valerate
1854 *para*-Menth-*3*-yl-*iso*-valerate
1693 "Menthylyl salicylate"
1430 "Meraneine"
1426 "Meranol"
2935 Mercaptoacetic acid
2934 *2*-Mercapto thiophene
1097 "Mertaste" (see also 1098)
1855 .... Mesitylene
1856 .... Mesityl oxide
431 Mesityl-*iso*-thiocyanate
1878 "Mesotan"
236 Metanethole
2653 Methacetone
2952 Methacide
1857 .... Methacrolein
1857 Methacrylaldehyde
1858 .... Methallyl acetal dihydropyran
1859 .... Methallyl butyrate
1860 .... Methallyl caproate
1861 .... Methallyl-*para*-methoxy phenylether
746 "*beta*-Methallyl mustard oil"
1830 Methane dicarboxylic acid
2099 Methane thiol
1410 Methanoic acid
1898 Methanol
2244 Methional
2245 Methionol
2244 *beta*-Methiopropional
1862 .... Methoxy acetic acid
13 *para*-Methoxy acetophenone
14 *3*-Methoxy-*4*-acetoxy-*1*-allylbenzol
15 Methoxy-*4*-acetoxy propenylbenzene
1131 *para*-Methoxy allylbenzene
1232 *2*-Methoxy-*4*-allylphenethole
1369 *2*-Methoxy-*4*-allylphenol
347 *2*-Methoxy-*6*-allylphenol
14 *2*-Methoxy-*4*-allyl-*1*-phenylacetate
1906 *ortho*-Methoxy amylbenzoate
1863 .... *para*-Methoxy-*alpha*-*n*-amylcinnamic aldehyde
1057 *2*-Methoxy anisaldehyde
256 *para*-Methoxy benzalacetone
1864 .... *ortho*-Methoxy benzaldehyde
241 *para*-Methoxy benzaldehyde
246 Methoxy benzene
245 *para*-Methoxy benzoic acid
284 *3*-Methoxy-*4*-benzoyloxy-*1*-allylbenzol
1865 .... *ortho*-Methoxy benzylacetate
247 *para*-Methoxy benzylacetate
248 *para*-Methoxy benzylacetone
249 *para*-Methoxy benzylalcohol
250 *para*-Methoxy benzylbenzoate
252 *para*-Methoxy benzylbutyrate
253 *para*-Methoxy benzyl-*iso*-butyrate
1286 *ortho*-Methoxy benzyl ethyl ether
254 *para*-Methoxy benzyl formate
255 *para*-Methoxy benzylheptanoate
256 *para*-Methoxy benzylidene acetone
313 *3*-Methoxy-*4*-benzyloxy propenylbenzene
260 *para*-Methoxy-*n*-benzyl-*n*-pentanoate

258 *para*-Methoxy benzyl phenylacetate
259 *para*-Methoxy benzyl propionate
2006 *2*-Methoxybiphenyl
1866 .... Methoxy-*iso*-chavibetol
1867 .... *para*-Methoxy cinnamic alcohol
1868 .... *ortho*-Methoxy cinnamic aldehyde
1869 .... *para*-Methoxy cinnamic aldehyde
1870 .... Methoxy citronellal
1871 .... *4*-Methoxy coumarin
2255 *7*-Methoxy coumarin (see also 3020)
2442 *5*-Methoxy-*ortho*-cresol
705 *2*-Methoxy-*para*-cresol
2947 *3*-Methoxy-*para*-cymene
1872 .... *6*-Methoxy dicyclopentadiene aldehyde
2102 "*3*-Methoxy dimethylanthranilate"
2097 *3*-Methoxy-*3*,*7*-dimethyl-*1*,*6*-octadiene
1870 *7*-Methoxy-*3*,*7*-dimethyloctan-*1*-al
2278 *4*-Methoxy-*1*,*3*-dinitro-*2*-methyl-*5*-*tertiary*-butylbenzene
1073 Methoxy-*iso*-divarinol
1862 Methoxy ethanoic acid
1222 *2*-Methoxy ethanol
1365 *3*-Methoxy-*4*-ethoxy benzaldehyde
1474 *1*-Methoxy-*3*-ethoxybenzene
1720 *1*-Methoxy-*4*-ethoxybenzene
1873 .... *3*-Methoxy-*4*-ethoxy methyl benzol
1873 *3*-Methoxy-*4*-ethoxy toluene
1284 *alpha*-Methoxy ethylbenzoate
1153 *para*-Methoxy ethylbenzoate
1287 *4*-Methoxy ethylcinnamate
1251 *2*-Methoxy-*4*-ethylphenol
1874 "*beta*-Methoxy ethylsalicylate"
1874 .... *para*-Methoxy ethylsalicylate
1538 *3*-Methoxy-*4*-heptoxy allylbenzene
1539 *3*-Methoxy-*3*-heptoxy propenylbenzene
1640 *para*-Methoxy hexylbenzoate
1875 .... *para*-Methoxy hydratropic aldehyde
28 *3*-Methoxy-*4*-hydroxy acetophenone
347 *1*-Methoxy-*2*-hydroxy-*4*-allylbenzol
1722 *1*-Methoxy-*4*-hydroxybenzene
3101 *3*-Methoxy-*4*-hydroxybenzylacetone
1880 *7*-Methoxy-*5*-hydroxy-*4*-methyl-coumarin
1695 *3*-Methoxy-*4*-hydroxy phenyl-acetaldehyde
3101 *4*-(*3*-Methoxy-*4*-hydroxyphenyl)-*2*-butanone
1747 *para*-Methoxy-*ortho*-hydroxyphenyl methyl ketone
2645 *2*-Methoxy-*1*-hydroxy-*6*-propenylbenzene
2645 *3*-Methoxy-*1*-hydroxy-*4*-propenylbenzene
2442 *3*-Methoxy-*5*-hydroxytoluene
1876 .... *4*-Methoxy-*3*-methyl benzaldehyde
717 *3*-Methoxy-*1*-methylbenzene
719 *4*-Methoxy-*1*-methylbenzene
1877 .... *ortho*-Methoxy methyl benzoate
1908 *para*-Methoxy methyl benzoate
2291 *3*-Methoxy-*4*,*5*-methylenedioxy allylbenzene
2028 *4*-Methoxy methylorsellinate
705 *2*-Methoxy-*4*-methylphenol
1878 .... Methoxy methylsalicylate
1879 .... *para*-Methoxy methylsalicylate
2155 *5*-Methoxy methylsalicylate
256 *para*-Methoxy methyl styryl ketone
2302 *2*-Methoxynaphthalene
1880 .... *7*-Methoxy-*5*-oxy-*4*-methylcoumarin
1472 *ortho*-Methoxyphenol
1722 *para*-Methoxyphenol
1477 *ortho*-Methoxyphenol phenylacetate
1881 .... *para*-Methoxy phenoxyacetaldehyde
1882 .... *para*-Methoxy phenylacetaldehyde
1475 *ortho*-Methoxy phenylacetate
1883 .... *para*-Methoxy phenylacetone
1476 *ortho*-Methoxy phenylbenzoate
1884 .... *ortho*-Methoxy-*4*-phenylbutanol-*2*
248 *para*-Methoxy phenylbutanone
1909 *2*-(*para*-Methoxyphenyl)-butan-*2*-one
377 *4*-(*para*-Methoxyphenyl)-*2*-butene
256 *4*-(*para*-Methoxyphenyl)-*3*-buten-*2*-one
1885 *2*-Methoxy-*1*-phenylethanol
1886 *para*-Methoxy phenylethyl acetone
1885 .... *2*-Methoxy-*2*-phenylethyl alcohol
1885 *ortho*-Methoxy phenylethylalcohol
1885 *para*-Methoxy phenylethylalcohol
1887 *ortho*-Methoxy phenylethyl ketone
1884 *ortho*-Methoxy phenylethyl methyl carbinol
1288 *para*-Methoxy phenylglycidic acid, ethylester
2936 *ortho*-Methoxy phenylmercaptan
1890 *1*-(*para*-Methoxyphenyl)-*4*-methyl-*1*-penten-*3*-one
2103 *3*-(*meta*-Methoxyphenyl)-methyl-propionate
2104 *3*-(*para*-Methoxyphenyl)-methyl-propionate
1886 *5*-(*4*-Methoxyphenyl)-pentan-*2*-one
1907 *1*-(*para*-Methoxyphenyl)-*1*-penten-*3*-one
237 *1*-(*para*-Methoxyphenyl)-propane-*2*-thiol
1887 *1*-(*ortho*-Methoxyphenyl)-*1*-propanone
1883 *1*-(*para*-Methoxyphenyl)-*2*-propanone
236 *para*-Methoxy-*alpha*-phenylpropene
1886 .... *alpha*-(*para*-Methoxyphenyl)-*n*-propyl methyl ketone
236 *1*-Methoxy-*4*-propenylbenzene
2644 *1*-Methoxy-*4*-*iso*-propenylbenzene
1866 *1*-Methoxy-*5*-propenylguaiacol
1370 *2*-Methoxy-*4*-propenylphenol
15 *2*-Methoxy-*4*-propenylphenyl acetate
1374 *2*-Methoxy-*4*-propenylphenyl formate
1376 *2*-Methoxy-*4*-propenylphenyl phenylacetate
1887 .... *ortho*-Methoxy propiophenone
944 *2*-Methoxy-*4*-propylphenol
2256 Methoxy resocyanin
2291 *5*-Methoxysafrole
1888 *3*-Methoxy salicylaldehyde
1888 .... *meta*-Methoxy salicylic aldehyde
1889 .... *para*-Methoxy salicylic aldehyde

1907 *para*-Methoxy styryl ethyl ketone
1890 .... *para*-Methoxystyryl-*iso*-propyl ketone
2936 *2*-Methoxy thiophenol
718 *ortho*-Methoxy toluene
719 *para*-Methoxy toluene
1876 *para*-Methoxy-*meta*-tolylaldehyde
1742 *5*-Methoxy vanillin
1891 .... *2*-Methoxy-*4*-vinyl phenol
1892 .... Methyl abietate
2652 Methyl acetaldehyde
1893 .... Methyl acetate
2654 Methyl acetic acid
1894 .... Methyl acetoacetate
1895 .... *para*-Methyl acetophenone
1736 *para*-Methyl acetophenone-hydroxycitronellal
44 *6*-Methyl-*3*-aceto-*2,4*-pyrandione
44 Methyl acetopyronone
1894 Methyl acetyl acetate
1895 Methyl acetyl benzene
1896 .... Methyl acetyl cyclopentane
1897 .... *2*-Methyl-*5*-acetyl pyridine
1857 *alpha*-Methyl acrolein
1397 Methylal
1898 .... Methyl alcohol
1859 *beta*-Methylallyl-*n*-butyrate
1860 *beta*-Methylallyl caproate
1860 *beta*-Methylallyl-*n*-hexoate
95 *1*-Methyl-*2*-allyl-*4*-*iso*-propylidene cyclohexanone-*2*
2100 Methylamine
1910 Methyl-*2*-aminobenzoate
493 *N*-Methylamino-*iso*-butylbenzoate
1899 .... *alpha*-Methyl-*alpha*-aminobutyric acid
2106 *2*-Methylamino methylbenzoate
1900 .... Methyl amylacetate
2040 Methyl amylacetic acid
2143 Methyl-*beta*-amylacrylate
1925 Methyl amylalcohol
2127 *alpha*-Methyl-*gamma*-amyl butyrolactone
1502 Methyl-*n*-amylcarbinol
1514 Methyl-*n*-amylcarbinyl acetate
1901 .... Methyl amyl catechol ketal
1749 *ortho*-Methyl-*para*-*tertiary*-amyl cyclohexanol
1902 .... *5*-Methyl-*6*-amyl-*5*-cyclohexen-*1*-one
2908 Methyl amyl cyclopentanone
1903 .... *3*-Methyl-*2*-*iso*-amyl cyclopentanone
954 Methyl-*3*-*n*-amyl-*2*-cyclopenten-*2*-one-*1*
955 Methyl-*3*-*iso*-amyl-*2*-cyclopenten-*2*-one-*1*
1904 .... Methyl-*delta*-amylenylcarbinol
492 "Methyl-*iso*-amylidene acetaldehyde"
1905 .... Methyl-*n*-amyl ketone
2993 Methyl-*n*-amylketone-*2,2*-dimethyl-*1,3*-propanediol ketal
2993 Methyl-*iso*-amylketone-*2,2*-dimethyl-*1,3*-propanediol ketal
2076 Methyl-(*2*-amyl-*3*-oxocyclopentyl)-acetate
1906 .... Methyl amyl salicylate
1907 .... *alpha*-Methyl anisalacetone
1908 .... Methyl anisate
1877 Methyl-*ortho*-anisate
1876 *meta*-Methyl anisic aldehyde
718 *ortho*-Methyl anisole
719 *para*-Methyl anisole
1907 *alpha*-Methyl anisylidene acetone
1909 .... *alpha*-Methyl anisyl ketone
2104 Methyl anisyl propionate
1910 .... Methyl anthranilate
1289 *N*-Methylanthranilic acid, ethylester
2171 *alpha*-Methyl-*alpha*-benzalacetone
1911 .... *para*-Methyl benzalacetophenone
2959 Methyl benzaldehyde, (mixed isomers)
2960 *meta*-Methyl benzaldehyde (*3*-Methyl-)
2961 *ortho*-Methyl benzaldehyde (*2*-Methyl-)
2962 *para*-Methyl benzaldehyde (*4*-Methyl-)
1595 *para*-Methyl benzaldehyde-di-*n*-hexathienyl acetal
2952 Methylbenzene
1912 .... Methyl benzoate
1999 *6*-Methyl benzodihydropyrone
1913 .... *ortho*-Methyl benzophenone
1965 *6*-Methyl benzopyrone
1914 .... *2*-Methyl benzoxazole
1915 .... Methyl benzyl acetate
2176 *alpha*-Methyl benzyl acetate
1915 *meta*-Methyl benzyl acetate (*3*-Methyl-)
2956 *para*-Methyl benzyl acetate (*4*-Methyl-)
1916 .... *alpha*-Methyl benzyl acetone
2967 *para*-Methyl benzyl acetone
2175 *alpha*-Methyl benzyl alcohol
2957 *ortho*-Methyl benzyl alcohol (*2*-Methyl-)
2958 *para*-Methyl benzyl alcohol (*4*-Methyl-)
2177 *alpha*-Methyl benzyl-*ortho*-aminobenzoate
2178 *alpha*-Methyl benzyl benzoate
2179 *alpha*-Methyl benzyl-*n*-butyrate
2180 *alpha*-Methyl benzyl-*iso*-butyrate
2181 *alpha*-Methyl benzyl caproate
1917 .... Methyl benzyl carbinol
1918 .... Methyl benzyl carbinyl acetate
2183 *alpha*-Methyl benzyl cinnamate
1919 .... Methyl benzyl ether
2071 Methyl benzyl ethylalcohol
2482 *6*-Methyl-*2*-benzyl-*1,3*-dioxan
2484 *5*-Methyl-*2*-benzyl-*1,3*-dioxolan
1703 *2*-(*alpha*-Methylbenzyl)-dioxolan
2184 *alpha*-Methyl benzyl formate
2181 *alpha*-Methyl benzyl hexanoate
2187 *alpha*-Methyl benzyl-*ortho*-hydroxybenzoate
1920 .... Methyl benzyl ketone
1921 .... *1*-*meta*-Methyl benzyl-*4*-methyl-*1,3*-dioxolan
1704 *2*-(*alpha*-Methylbenzyl)-*5*-methyl-*1,3*-dioxolan

2182 *alpha*-Methyl benzyl octanoate
2188 *alpha*-Methyl benzyl-*iso*-pentanoate
2185 *alpha*-Methyl benzyl phenylacetate
1922 .... *meta*-Methyl benzyl propionate
1923 .... *para*-Methyl benzyl propionate
1938 *2*-Methylbutanal-*1* (see also 3053)
3053 *2*-Methylbutanal-*4*
3053 *3*-Methylbutanal-*1*
2266 *2*-Methylbutane-*1*-carboxylic acid
2267 *3*-Methylbutane-*1*-carboxylic acid
1059 Methylbutane dioate
1939 Methyl-*n*-butanoate
1941 *2*-Methylbutanoic acid
1674 *2*-Methylbutanoic acid, *n*-hexylester
127 *alpha*-Methylbutanol
126 *gamma*-Methyl-*n*-butanol
1424 *2*-Methylbutanol-*1*
1008 *2*-Methylbutanol-*2*
1424 *2*-Methylbutanol-*4*
126 *3*-Methyl-*1*-butanol
119 *2*-Methylbutanol-*1*-acetate
121 *2*-Methylbutanol-*2*-acetate
132 *3*-Methyl-*1*-butanol benzoate
2227 *2*-Methyl-*3*-butanone
984 *3*-Methylbuten-*2*-al-*1*
1968 Methyl-*trans*-*2*-butenoate
238 *cis*-*2*-Methyl-*2*-butenoic acid
2949 *trans*-*2*-Methyl-*2*-butenoic acid
2640 *2*-Methylbuten-*2*-ol-*4*
1924 .... *2*-Methyl-*3*-buten-*2*-ol
985 *3*-Methylbuten-*2*-ol-*1*
2641 *2*-Methylbuten-*2*-ol-*4*-acetate
2951 *trans*-*2*-Methylbutenoyl piperidide
2394 Methyl butenyl propenol
120 *alpha*-Methyl butyl acetate
1946 Methyl-*iso*-butyl acetate
119 *3*-Methyl-*1*-butyl acetate
139 *alpha*-Methyl butyl butyrate
1925 .... Methyl-*iso*-butyl carbinol
1900 Methyl-*iso*-butyl carbinyl acetate
1926 .... Methyl-*iso*-butyl carbinyl ethylether
1665 Methyl-*n*-butyl carbinyl-*2*-furoate
1927 .... Methyl butyl catechol ketal
1928 .... *ortho*-Methyl-*para*-*tertiary*-butyl cyclohexanol
1929 .... *ortho*-Methyl-*para*-*tertiary*-butyl cyclohexanyl acetate
1930 .... *3*-Methyl-*iso*-butyl-*2*-furylketone
1931 .... *5*-Methyl-*3*-*iso*-butyl-*3*-hexanol
495 *alpha*-Methyl-*para*-*iso*-butyl hydrocinnamic aldehyde
496 *alpha*-Methyl-*para*-*tertiary*-butyl hydrocinnamic aldehyde
1932 .... *3*-Methyl-*5*-*n*-butylidene cyclopenten-*2*-one-*1*
1933 .... Methyl-*iso*-butyl ketone
2014 Methyl-*secondary*-butyl ketone
2618 Methyl-*tertiary*-butyl ketone
430 Methyl-*4*-*tertiary*-butyl-*3*-methoxybenzene
1799 Methyl-*N*-(*para*-*tertiary*-butyl)-*alpha*-methylhydrocinnamylidene anthranilate
429 *3*-Methyl-6-*tertiary*-butylphenol
1934 .... Methyl-*para*-*tertiary*-butyl phenylacetate
495 *2*-Methyl-*3*-(*para*-*iso*-butylphenyl)-*1*-propanal
496 *alpha*-Methyl-*beta*-(*para*-*tertiary*-butylphenyl)-propionaldehyde
1935 .... *5*-Methyl-*3*-butyl tetrahydropyran-*4*-yl acetate (see also 2346)
1936 .... *2*-Methylbutyl-*iso*-valerate
1937 .... *2*-Methyl butynol
1938 .... *alpha*-Methyl butyraldehyde
3053 *2*-Methyl-*n*-butyraldehyde
1939 .... Methyl butyrate
1940 .... Methyl-*iso*-butyrate
1941 .... *alpha*-Methyl butyric acid
3057 *beta*-Methyl butyric acid
3057 *3*-Methyl butyric acid
1942 .... Methyl-*iso*-butyryl acetone
1943 .... Methyl-*iso*-campholate
1944 Methyl caprate
1944 .... Methyl caprinate
1945 .... Methyl caproate
1946 .... Methyl-*iso*-caproate
1947 .... Methyl caprylate
903 Methyl carbitol (see also 905)
998 Methyl carbonate
1948 .... Methyl carbostyril
1472 Methyl catechol
599 Methyl cedrylether
1222 Methyl cellosolve
1126 *beta*-Methyl chalkone
2646 Methyl-*iso*-chavibetol
1131 Methyl chavicol
58 Methyl chrysanthemumate
1951 *alpha*-Methyl cinnamal
1949 .... Methyl cinnamate
1950 .... *alpha*-Methyl cinnamic alcohol (see also 1691)
1950 *beta*-Methyl cinnamic alcohol
1951 .... *alpha*-Methyl cinnamic aldehyde
1951 *beta*-Methyl cinnamic aldehyde
1952 .... *alpha*-Methylcinnamic aldehyde diethyl acetal
1953 .... *alpha*-Methylcinnamic aldehyde dimethyl acetal
1954 .... *alpha*-Methyl cinnamyl acetate
1954 *beta*-Methyl cinnamyl acetate
1691 Methylcinnamylidene carbinol
1955 .... *alpha*-Methylcinnamylidene methylanthranilate
2171 *alpha*-Methylcinnamylidene methylketone
640 *1*-Methyl-*2*-cinnamylidene-*4*-*iso*-propylidene cyclohexan-*3*-one
318 Methyl cinnamyl ketone
1956 .... *3*-Methyl citral
1956 "Methyl-*3*-citral"
1957 .... Methyl citrate
1958 .... *3*-Methyl citronellal
1958 *3*-Methyl-*beta*-citronellal
1959 .... Methyl citronellate
1960 .... Methyl citronellol
1961 .... Methyl citronellyl ether
1962 *alpha*-Methylcoumarin

1963 *beta*-Methylcoumarin
1962 .... *3*-Methyl coumarin
1963 .... *4*-Methyl coumarin
1964 .... *5*-Methyl coumarin
1965 .... *6*-Methyl coumarin
1966 .... *7*-Methyl coumarin
1967 .... *8*-Methyl coumarin
719 Methyl-*para*-cresol
2118 Methyl-*meta*-cresotinate
1195 Methyl-*para*-cresylacetal
719 Methyl-*para*-cresylate
2950 *alpha*-Methyl crotonaldehyde
984 *beta*-Methyl crotonaldehyde
1968 .... Methyl crotonate
238 *cis-alpha*-Methylcrotonic acid
238 *cis-2*-Methylcrotonic acid
2949 *trans-alpha*-Methylcrotonic acid
2949 *trans-2*-Methylcrotonic acid
239 *gamma*-Methyl-*alpha-beta*-crotonolactone
239 *gamma*-Methyl-*beta-gamma*-crotonolactone
985 *3*-Methyl crotylalcohol
2220 *2*-Methyl-*3*-cumenylpropanol
21 Methyl cyanide
1969 .... Methyl cyclocitrylidene acetate
1970 .... *2*-Methyl cyclohexanone
1971 .... *3*-Methyl cyclohexanone
1972 .... *4*-Methyl cyclohexanone
2928 *4*-Methyl-*3*-cyclohexene aldehyde
1974 *3*-(*4*-Methyl-*3*-cyclohexenyl)-butanal
1973 .... *4*-(*1*-Methyl-*3*-cyclohexenyl)-*3*-buten-*2*-one
1974 .... *beta*-(*4*-Methyl-*3*-cyclohexenyl)-butyraldehyde
1981 Methyl cyclohexenyl methyl carbinyl acetate
1975 .... *1*-(*6*-Methyl-*3*-cyclohexenyl)-*1*-penten-*2*-one
1976 .... *2*-Methyl cyclohexyl acetate
1977 .... *4*-Methyl cyclohexyl acetate
1979 *3*-(*para*-Methyl cyclohexyl)-butanal
1978 .... *beta*-(*4*-Methyl cyclohexyl)-butanol
1979 .... *beta*-(*4*-Methyl cyclohexyl)-butyraldehyde
1980 .... *para*-Methyl cyclohexyl ethylether
36 Methyl cyclohexyl ketone
1981 .... *4*-Methyl cyclohexyl methyl carbinyl acetate
1743 *4*-Methyl-*4*-cyclohexyl pentan-*2*-ol
803 *2*-Methyl-*2*-cyclohexyl propan-*1*-ol
1982 .... *1*-Methyl cyclopentadecan-2-one
2276 *3*-Methyl cyclopentadecanone-*1*
2276 *beta*-Methyl cyclopentadecanone
1983 .... *4*-Methyl cyclopentadecanone-*1*
1984 .... *5*-Methyl cyclopentadecanone-*1*
1985 .... *3*-Methyl cyclopentadecenone
1987 *3*-Methyl cyclopentane-*1*,*2*-dione
1986 .... Methyl cyclopentanol
1986 *1*-Methyl cyclopentan-*1*-ol
1992 *2*-Methyl cyclopent-*1*-ene-*1*-acetic acid, ethylester
1987 .... Methyl cyclopentenolone
1988 .... Methyl cyclopentenolone butyrate
1989 .... Methyl cyclopentenolone-*3*,*4*-dioxy-*5*-methoxy-*iso*-propyl benzene
1990 .... Methyl cyclopentenolone propionate
1991 .... Methyl cyclopentenyl acetate
1991 *2*-Methyl cyclopentenyl acetate
1992 .... Methyl cyclopentenyl ethylacetate
1986 Methyl cyclopentyl alcohol
1993 .... *4*-Methyl cyclotetradecan-*1*-one
1994 .... Methyl Decahydro naphthyl acetate
2145 *2*-Methyl decanal
1944 Methyl decanoate
1995 .... Methyl-*2*-decenoate
2078 Methyl decenolide-*1* : *4*
1996 .... Methyl decincarbonate
1997 .... Methyl decyl acetaldehyde
1944 Methyl decylate
1995 Methyl-*2*-decylenate
1998 .... Methyl decyl ketone
2131 Methyl decynoate
2202 Methyl dihydrocinnamate
1999 .... *6*-Methyl dihydrocoumarin
2000 .... Methyl dihydroeugenol
2076 Methyl dihydrojasmonate
2001 .... *2*-Methyl-*3*,*4*-dihydroxy-*4*-ethyl-5-oxotetrahydrofuran
2441 *1*-Methyl-*3*,*5*-dimethoxybenzene
2943 *2*-Methyl-*1*,*4*-dimethoxy-*5*-*iso*-propylbenzene
1940 Methyl dimethylacetate
2002 .... Methyl-*N*,*N*-dimethylanthranilate
2003 .... *para*-Methyl dimethylbenzyl carbinol
2998 *1*-Methyl-*3*,*3*-dimethyl cyclohexanol-*5*
2004 .... Methyl-*3*,*5*-dimethyl-*2*,*3*-epoxy-*4*-hexenoate
2111 Methyl-*3*,*7*-dimethyl-*2*,*3*-epoxy-*6*-octenoate
1735 Methyl-*N*-*3*,*7*-dimethyl-7-hydroxy-octylidene anthranilate
2005 .... Methyl dimethylmalonate
2006 .... Methyl diphenylether
2493 Methyl diphenylketone
2007 .... Methyl diphenyl methane
1006 Methyl disulfide
2007 *alpha*-Methyl ditane
2003 *para*-Methyl D.M.B.C.
1391 *3a*-Methyl dodecahydro-*6*,*6*,*9a*-trimethylnaphtho-(*2*,*1*-*b*)-furan
1997 *alpha*-Methyl dodecanal
2141 *3*-Methyldodecanal-*1*
2095 Methyl dodecanoate
1997 *10*-Methyl dodecylaldehyde
2095 Methyl dodecylate
2260 Methyl-*2*-dodecynoate
2269 Methylene acetone
2008 .... *3*-Methylene-*4*-bornylbutanol
2009 .... *alpha*-Methylene citronellal
2270 Methylene citronellol
1985 *3*-Methylene cyclopentadecanone
1395 Methylene dibutylether
1396 Methylene diethylether
1779 *4*-(*2*-Methylene-*6*,*6*-dimethylcyclohexenyl)-*3*-buten-*2*-one
950 *4*-(*2*-Methylene-*6*,*6*-dimethyl-cyclohexyl)-butan-*2*-one

2090 *4*-(*2*-Methylene-*6*,*6*-dimethylcyclohexyl)-*3*-methyl-*3*-buten-*2*-one
2089 *5*-(*2*-Methylene-*6*,*6*-dimethylcyclohexyl)-*4*-penten-*3*-one
1397 Methylene dimethylether
2009 *2*-Methylene-*3*,*7*-dimethyl-*6*-octen-*1*-al
2010 .... *3*,*4*-Methylene dioxyacetophenone
2813 *3*,*4*-Methylene dioxyallyl benzene
975 *1*,*2*-Methylenedioxy-*4*-allyl-*5*,*6*-dimethoxybenzene
2011 .... *3*,*4*-Methylenedioxy-*alpha*-*n*-amylcinnamic aldehyde
1484 *3*,*4*-Methylenedioxy benzaldehyde
591 *1*,*2*-Methylene dioxybenzene
2632 *3*,*4*-Methylenedioxy benzoic acid
1487 *3*,*4*-Methylenedioxy benzylacetate
1488 *3*,*4*-Methylenedioxy benzylacetone
1489 *3*,*4*-Methylenedioxy benzylalcohol
1491 *3*,*4*-Methylenedioxy cinnamic aldehyde
1692 *3*,*4*-Methylenedioxy phenylacetaldehyde
1488 *4*-(*3*,*4*-Methylenedioxyphenyl)-*2*-butanone
604 *3*,*4*-Methylenedioxy phenylpentadienoic acid (see also 605)
976 *1*,*2*-Methylenedioxy-*4*-propenyl-*5*,*6*-dimethoxybenzene
968 *3*,*4*-Methylenedioxy propylbenzene
2814 *1*,*2*-Methylenedioxy-*4*-propylene benzene
2814 *3*,*4*-Methylenedioxy-*1*-propylene benzene
1398 Methylene dipropylether
964 *3*-Methylene-7-methyloctanol-7
965 *3*-Methylene-7-methyloctan-7-yl acetate
2284 *3*-Methylene-7-methyl-*1*-octen-7-ol
2285 *3*-Methylene-7-methyl-*1*-octen-*7*-yl acetate
2286 *3*-Methylene-7-methyl-*1*-octen-7-yl formate
2287 *3*-Methylene-7-methyl-*1*-octen-7-yl propionate
2811 *4*-Methylene-*1*-*iso*-propylbicyclo-(*0* : *1* : *3*)-hexanol-*5*
2460 *1*-Methylene-*4*-*iso*-propyl-*2*-cyclohexene
2024 *para*-Methyl-E.P.G.
196 *beta*-Methyl-*alpha*-*beta*-epoxyacetic acid, amylester
2023 Methyl-*2*,*3*-epoxy-*3*-ethylhydrocinnamate
2193 Methyl-*alpha*-*beta*-epoxy hydrocinnamate
2117 Methyl-*alpha*-*beta*-epoxy-*beta*-methylhydrocinnamate
1783 Methyl-*2*,*3*-epoxy-*3*-methyl-*5*-(*2*,*6*,*6*-trimethyl-*2*-cyclohexenyl)-*4*-pentenoate
2193 Methyl-*alpha*-*beta*-epoxy phenylpropionate
1893 Methyl ethanoate
2012 .... Methyl-*ortho*-ethoxybenzoate
2013 .... *4*-Methyl-*7*-ethoxycoumarin
2946 *1*-Methyl-*3*-ethoxy-*4*-*iso*-propylbenzene
2012 Methyl-*beta*-ethoxysalicylate
1938 Methyl ethyl acetaldehyde
1941 Methyl ethyl acetic acid
1292 Methyl ethyl acetic acid, ethylester
2014 .... Methyl ethyl acetone
2015 .... *alpha*-Methyl-*beta*-ethyl acrolein
2016 .... Methyl ethyl benzyl carbinol
2017 .... Methyl ethyl benzyl carbinyl acetate
391 Methyl ethyl carbinol
459 Methyl ethyl carbinyl furan-*2*-carboxylate
459 Methyl ethyl carbinyl pyromucate
2001 Methyl ethyl dihydroxy tetrahydrofuranone
2018 .... Methyl ethyl-*iso*-eugenol
2649 "Methyl ethyl-*iso*-eugenol"
1271 Methyl ethyl glycollic acid, ethylester
2019 .... Methyl-*3*-ethyl heptenone
1253 Methyl ethyl hexenone
766 *alpha*-Methyl ethyl ionone
2020 .... Methyl ethyl ketone
2541 Methyl ethyl phenethyl carbinol
2021 .... Methyl ethyl phenyl carbinol
2022 .... Methyl ethyl phenyl carbinyl acetate
2541 Methyl ethyl phenyl ethyl carbinol
2542 Methyl ethyl phenyl ethyl carbinyl acetate
2544 Methyl ethyl phenylethyl carbinyl-*iso*-pentanoate
2543 Methyl ethyl phenylethyl carbinyl propionate
2023 .... Methyl ethyl phenylglycidate
2024 .... *para*-Methyl ethyl phenyl glycidate
2025 .... *3*-Methyl-*4*-ethyl pyridine
1308 *4*-Methyl-*3*-ethyl pyridine
2276 Methyl exaltone
2026 .... Methyl eugenol
2027 .... Methyl-*iso*-eugenol
2028 .... Methyl everninate
980 Methyl ferulaldehyde
2029 .... Methyl formate
3005 Methyl-*ortho*-formate
2031 *5*-Methyl-*2*-furaldehyde
2034 *alpha*-Methyl furanacrolein
239 *5*-Methyl-*2*,*3H*-furanone
239 *5*-Methyl-*2*,*5H*-furanone
2032 Methyl-*2*-furanpropionate
2034 *alpha*-Methyl furfuracrolein
2030 .... Methyl furfuracrylate
2031 .... *alpha*-Methyl furfural
2031 *5*-Methyl furfural
2032 .... Methyl furfurhydracrylate
2031 Methyl furfurol-(*2*,*5*)
2033 .... Methyl furoate
2034 *alpha*-Methyl-*beta*-*2*-furylacraldehyde
2034 .... *alpha*-Methyl-*beta*-furyl acrolein
2030 Methyl-*beta*-furylacrylate
39 Methyl-*alpha*-furyl ketone
2034 *2*-Methyl-*3*-(*2*-furyl)-propenal
2032 Methyl furyl propionate
2155 Methyl gentisate-*5*-methylether

2035 .... Methyl geraniol
2647 "Methyl-*iso*-geraniol"
2648 "Methyl-*iso*-geranyl acetate"
2036 .... Methyl geranoxy acetate
2037 .... Methyl geranyl ether
769 Methyl geranyl ketone
2038 .... Methyl geranyl tiglate
2696 "Methyl glycol"
2786 Methyl glyoxal
705 *4*-Methyl guaiacol
2132 *2*-Methyl hendecanal
2257 Methyl hendecanoate
2393 *4*-Methyl-*2*,*4*-heptadien-*1*-al
2394 *4*-Methyl-*2*,*4*-heptadien-*1*-ol
2039 .... *2*-Methylheptadien-(*2*,*4*)-one-*6*
2039 *6*-Methylheptadien-*3*,*5*-one-*2*
2046 Methyl heptanoate
2040 .... *2*-Methyl heptanoic acid
1146 *2*-Methyl-*5*-heptanol
2058 *6*-Methylheptanol-*2*
1146 *6*-Methyl-*3*-heptanol
2041 .... *2*-Methylheptanol-*6*-acetate (see also 2405)
1148 *5*-Methyl-*3*-heptanone
2067 *6*-Methylheptan-*2*-one
1149 *6*-Methyl-*3*-heptanone
1147 *6*-Methylheptan-*3*-yl acetate
2042 .... Methyl heptenol
393 *6*-Methyl-*1*-hepten-*4*-ol
2043 .... *2*-Methylheptenone
2043 *2*-Methyl-*1*-hepten-*6*-one
2043 *2*-Methyl-*2*-hepten-*6*-one
2044 .... Methyl heptenyl acetate
2358 Methyl heptenyl ketone
2045 .... Methyl heptin carbonate
2114 Methyl heptin carbonate (see also 2148, 2149, 2150, 2151 and 2152)
2046 .... Methyl heptoate
2047 .... Methyl heptyl acetaldehyde
1995 Methyl-*beta*-heptylacrylate
2046 Methyl heptylate
2048 .... Methyl heptyl carbinol
2364 Methyl heptyl carbinyl acetate
2049 .... *3*-Methyl-*2*-*n*-heptyl cyclopentan-*1*-one
2050 .... Methyl heptylene carbinol
2051 .... Methyl heptyl ether
1549 Methyl-*N*-heptylidene anthranilate
2052 .... Methyl heptyl ketone
2045 Methyl-*n*-hept-*1*-yne carboxylate
2116 Methyl heptynoate
2055 Methyl-2-heptynoate
2997 Methyl hexahydro-*2*,*4*-dimethyl phenyl carbinyl acetate
2724 *beta*-Methyl hexahydro homocuminic alcohol
48 *5*-Methyl-*2*,*3*-hexane dione
1945 Methyl hexanoate
1170 *2*-Methylhexan-*4*-yl-*iso*-butyrate
388 *6*-Methylhexen-*2*-al-*1*
2053 .... Methyl-*2*-hexenoate
2054 .... Methyl hexenyl ether
2043 Methyl hexenyl ketone
2055 .... Methyl hexin carbonate (see also 2116)
1945 Methyl hexoate
2056 .... Methyl hexyl acetaldehyde
1515 *2*-Methyl hexyl acetate
1945 Methyl hexylate
2057 .... Methyl hexyl carbinol
2058 .... Methyl-*iso*-hexyl carbinol
2405 Methyl-*n*-hexyl carbinyl acetate
2041 Methyl-*iso*-hexyl carbinyl acetate
2413 Methyl hexyl carbinyl-*iso*-butyrate
2059 .... *alpha*-Methyl-*n*-hexyl carbinyl formate
2434 Methyl hexyl carbinyl phenylacetate
2434 Methyl hexyl carbinyl-*alpha*-toluate
2060 .... *3*-Methyl-*4*-*iso*-hexyl cyclohexanol
2060 .... *3*-Methyl-*6*-hexyl cyclohexanol
2061 .... Methyl-*2*-*iso*-hexyl-*4*-cyclohexanone-*1*
2062 .... Methyl-*4*-*iso*-hexyl-*2*-cyclohexanone
2063 .... Methyl-*5*-*iso*-hexyl-*2*-cyclohexanone
2064 .... Methyl-*3*-hexyl-*2*-cyclopenten-*2*-one-*1*
1675 *5*-Methyl-*2*-hexyl-*1*,*3*-dioxolane
2065 .... Methyl-*n*-hexylether
592 Methyl hexyl ketal
2066 .... Methyl hexyl ketone
2067 .... Methyl-*iso*-hexyl ketone
2993 Methyl hexyl ketone-*2*,*2*-dimethyl-*1*,*3*-propanediol ketal
2068 .... *3*-Methyl hexyl methacrylate
2136 *beta*-Methyl-*beta*-hexyl propionaldehyde
2167 Methyl hexynoate (see also 2107)
2069 .... Methyl homovanillin
2070 .... *para*-Methyl hydratropic aldehyde
2203 Methyl hydratropyl ether
2202 Methyl hydrocinnamate
2071 .... *2*-Methyl hydrocinnamic alcohol
3100 *meta*-Methyl hydrocinnamic alcohol
2072 .... *alpha*-Methyl hydrocinnamic aldehyde
2073 .... *para*-Methyl hydrocinnamic aldehyde
2074 .... *alpha*-Methyl hydrocinnamic aldehyde dimethyl acetal
2075 .... *alpha*-Methyl hydrocinnamyl acetate
2203 Methyl hydrocinnamyl ether
328 Methyl hydrocinnamyl ketone
1999 *6*-Methyl hydrocoumarin
2076 .... Methyl hydrojasmonate
2953 *2*-Methylhydroquinone dimethylether
2081 *3*-Methyl-*2*-hydroxy acetophenone
2077 .... *3*-Methyl-*6*-hydroxy acetophenone
1754 *4*-(*4*-Methyl-*4*-hydroxyamyl)-*3*-cyclohexene carboxaldehyde
1754 *4*-(*4*-Methyl-*4*-hydroxyamyl)-*4*-cyclohexene carboxaldehyde
707 *1*-Methyl-*3*-hydroxybenzene
708 *1*-Methyl-*4*-hydroxybenzene
2241 Methyl-*ortho*-hydroxybenzoate
245 Methyl-*para*-hydroxybenzoate
1231 *alpha*-Methyl-*alpha*-hydroxybutanoic acid, ethylester
2079 Methyl-*3*-hydroxycaproate
2255 *4*-Methyl-*7*-hydroxycoumarin
1986 *2*-Methyl hydroxycyclopentane

2078 .... *4*-Methyl-*4*-hydroxy-*7*-decenoic acid, lactone
43 Methyl-*1*-hydroxyethyl ketone
2079 .... Methyl-*3*-hydroxyhexanoate
2028 Methyl-*6*-hydroxy-*2*-methylanisate
2080 .... Methyl-*N*-(*4*-(*4*-hydroxy-*4*-methylpentyl)-*3*-cyclohexenyl methylidene))-anthranilate
2081 .... *meta*-Methyl-*ortho*-hydroxymethyl phenylketone
2239 Methyl-*12*-hydroxy-*9*-octadecenoate
2016 *2*-Methyl-*2*-hydroxy-*1*-phenylbutane
1301 *alpha*-Methyl-*alpha*-hydroxypropionic acid, ethylester
2944 *1*-Methyl-*3*-hydroxy-*4*-*iso*-propylbenzene
2245 Methyl-*3*-hydroxy propyl sulfide
1948 *4*-Methyl-*2*-hydroxyquinoline
2118 Methyl-*2*-hydroxy-*para*-toluate
2082 .... *alpha*-Methyl indole
2846 *beta*-Methyl indole
2846 *3*-Methyl indole
2083 .... *5*-Methyl indole
2084 .... *alpha*-Methyl ional
2085 .... *alpha*-*n*-Methyl ionone
2086 .... *alpha*-*iso*-Methyl ionone
2087 .... *beta*-*n*-Methyl ionone
2088 .... *beta*-*iso*-Methyl ionone
2088 *delta*-Methyl ionone
2086 "*gamma*"-Methyl ionone
2089 .... *gamma*-*n*-Methyl ionone
2090 .... *gamma*-*iso*-Methyl ionone
2086 *iso*-Methyl-*alpha*-ionone
2088 *iso*-Methyl-*beta*-ionone
2091 .... *4*-Methyl ionone
2092 .... *5*-Methyl ionone
2092 *5*-Methyl-*alpha*-ionone
1784 *6*-Methyl-*alpha*-ionone
2092 *5*-Methyl-*beta*-ionone
1785 *6*-Methyl-*beta*-ionone
1786 *6*-Methyl-*gamma*-ionone
1783 Methyl-*alpha*-ionone glycidate
2084 Methyl ionyl acetaldehyde
2093 .... Methyl jasmonate
2094 .... Methyl-*iso*-jasmonate
2095 .... Methyl laurate
2096 .... Methyl linalool
2097 "Methyl linalool"
2096 *3*-Methyl linalool (see also 2097)
1817 *N*-Methyl linalyl anthranilate
2097 .... Methyl linalyl ether
2098 .... Methyl malonate
911 Methyl malonic acid, diethylester
2005 Methyl malonic acid, dimethylester
911 "Methyl malonic ester"
1999 "Methyl melilotine"
2099 .... Methyl mercaptan
2100 .... *4*-Methyl mercaptobutylamine
2100 *4*-Methyl mercaptobutyraldehyde
2120 Methyl mercapto methylpropionate
2244 Methyl-*beta*-mercaptopropionaldehyde
2245 *gamma*-Methyl mercaptopropylalcohol
2029 Methyl methanoate
1877 Methyl-*ortho*-methoxybenzoate
1908 Methyl-*para*-methoxybenzoate
256 Methyl-*para*-methoxycinnamyl ketone
2256 *4*-Methyl-*7*-methoxycoumarin
2101 .... *1*-Methyl-*3*-methoxy-*4*,*6*-di-tertiary-bytyl-*2*,*5*-dinitrobenzene
2103 Methyl-*meta*-methoxy-hydrocinnamate
2104 Methyl-*para*-methoxy-hydrocinnamate
2102 .... Methyl-*3*-methoxy-*2*-methylaminobenzoate
1875 *alpha*-Methyl-*para*-methoxyphenylacetaldehyde
2103 .... Methyl-(*meta*-methoxyphenyl)-propionate
2104 .... Methyl-(*para*-methoxyphenyl)-propionate
2947 *1*-Methyl-*3*-methoxy-*4*-*iso*-propylbenzene
2105 .... *5*-Methyl-*7*-methoxy-*8*-*iso*-propyl-*alpha*-tetralone
2102 Methyl-*2*-methylamino-*3*-methoxybenzoate
2106 .... Methyl-*N*-methyl anthranilate
2246 Methyl-*para*-methyl benzoate
2246 *para*-Methyl methylbenzoate
2108 Methyl-*2*-methylbutanoate
2004 Methyl methyl-*secondary*-butenylglycidate
2107 .... Methyl-*3*-methyl-*n*-but-*1*-yne carbonate
2108 .... Methyl-*2*-methylbutyrate
2264 Methyl-*3*-methylbutyrate
1955 Methyl-*N*-*alpha*-methylcinnamylidene anthranilate
2109 .... *5*-Methyl-*1*-(*3*-methyl-*3*-cyclohexenyl)-*1*,*3*-hexanedione
2916 Methyl-*para*-methyl cyclohexenyl ketone
2205 Methyl-*3*,*4*-methylenedioxybenzoate
2110 .... *alpha*-Methyl-*3*,*4*-methylenedioxy hydrocinnamic aldehyde
2283 *7*-Methyl-*3*-methylene-*1*,*6*-octadiene
2284 *2*-Methyl-*6*-methylene-*7*-octen-*2*-ol
2285 *2*-Methyl-*6*-methylene-*7*-octen-*2*-yl acetate
2286 *2*-Methyl-*6*-methylene-*7*-octen-*2*-yl formate
2287 *2*-Methyl-*6*-methylene-*7*-octen-*2*-yl propionate
2843 *10*-Methyl-*1*-methylene-*7*-*iso*-propenyl decahydronaphthalene
2108 Methyl methylethyl acetate
2111 .... Methyl methylheptenone glycidate
2112 .... Methyl-*6*-methyl-*n*-hept-*5*-en-yne carbonate
2113 .... Methyl-*6*-methyl-*n*-hept-*1*-yne carbonate
2114 .... Methyl-*5*-methyl-*n*-hex-*1*-yne carbonate
2005 Methyl methylmalonate
2120 Methyl-*2*-methyl mercaptopropionate
1946 Methyl-*4*-methylpentanoate
2115 .... *1*-Methyl-*4*-(*4*-methyl-*3*-pentenyl)-*3*-cyclohexene carboxaldehyde

2116 .... Methyl-*4*-methyl-*n*-pent-*1*-yne carbonate
2070 *para*-Methyl-*alpha*-methyl phenylacetaldehyde
2117 .... Methyl methylphenyl glycidate
1974 *1*-Methyl-*para*-(*3*-methylpropanal)-*1*-cyclohexene
1940 Methyl-*2*-methylpropanoate
2118 .... *6*-Methyl-*4*-(*3*-methylpropenyl-*5*-octen-*2*-one
2119 Methyl-*para*-methylsalicylate
2119 .... *para*-Methyl methylsalicylate
2120 .... Methyl-*beta*-methyl thiolpropionate
2135 Methyl-*N*-(*2*-methylundecenylidene)-anthranilate
1946 Methyl-*4*-methylvalerate
2121 .... Methyl myristate
2122 .... Methyl-*beta*-naphthyl acetaldehyde
2302 Methyl-*beta*-naphthylether
2123 .... *alpha*-Methyl naphthyl ketone
2124 .... *beta*-Methyl naphthyl ketone
2125 .... Methyl nahpthyl ketone – methylanthranilate
2126 .... Methyl nicotinate
2338 *1*-Methyl-*2*-nitrobenzene
2127 .... Methyl-*gamma*-nonalactone
2127 *2*-Methyl-*1* : *4*-nonalactone
2047 *2*-Methyl nonanal
2136 *3*-Methyl nonanal
2136 *7*-Methyl nonanal
2128 .... Methyl nonanoate
2129 .... Methyl-*8*-nonen-*2*-al-*1*
2130 .... *3*-Methyl-*2*-nonene nitrile
2139 Methyl-*2*-nonenoate
2427 Methyl nonenyl ketone
2112 Methyl nonenynoate
2131 .... Methyl nonin carbonate
2132 .... Methyl nonyl acetaldehyde
2133 .... Methyl nonyl acetaldehyde diethyl acetal
2134 .... Methyl nonyl acetaldehyde dimethyl acetal
2135 .... Methyl nonyl acetaldehyde-methylanthranilate
849 Methyl-*n*-nonylacetate
2136 .... *7*-Methyl nonylaldehyde
2136 "*7*-Methyl nonyl aldehyde" (see also 2056)
2136 *beta*-Methyl nonyl aldehyde
2128 Methyl nonylate
2137 .... Methyl nonyl carbinol
2138 .... Methyl nonyl carbinyl acetate
2139 .... Methyl nonylenate
2140 .... Methyl nonyl ketone
2195 Methyl nonyl phenyl carbinol
2141 *beta*-Methyl nonyl propanal
2141 .... Methyl nonyl propionic aldehyde
2113 Methyl nonynoate (see also 2144)
2242 Methyl octadecanoate
2153 *cis*-Methyl-*9*-octadecenoate
2056 *2*-Methyl octanal
1947 Methyl octanoate
2142 .... *7*-Methyloctanolide-*1* : *4*
567 *7*-Methyloct-*5*-ene-*1*-carboxylic acid, vanillylamide
2143 .... Methyl-*2*-octenoate
1253 *6*-Methylocten-*5*-one-*2*
2130 *2*-Methyl-*1*-octen-*1*-yl cyanide
2144 .... Methyl octin carbonate (see also 2113)
1947 Methyl octoate
2145 .... Methyl octyl acetaldehyde
1947 Methyl octylate
2143 Methyl-*2*-octylenate
2147 Methyl octyl glycolate
2146 .... Methyl octyl ketone
2147 .... Methyl octyl-*2*-oxyacetate
2144 Methyl octyne carboxylate
2114 Methyl octynoate
2045 Methyl-*2*-octynoate
2148 .... Methyl-*3*-octynoate
2149 .... Methyl-*4*-octynoate
2150 .... Methyl-*5*-octynoate
2151 .... Methyl-*6*-octynoate
2152 .... Methyl-*7*-octynoate
2381 *3*-Methyl-*1*-octyn-*3*-ol acetate
2046 "Methyl oenanthate"
2040 *2*-Methyl oenanthic acid
1862 Methyloglycolic acid
2153 .... Methyl oleate
2404 Methylol methyl amyl ketone
2352 Methylol methyl hexyl ketone acetate
1169 *3*-Methylolpentane acetate
1649 *alpha*-(*3*-Methylolpentane)-*gamma*-butyrolactone
1171 *3*-Methylolpentane cyclohexylacetate
2154 .... Methyl oxalate
248 "Methyl oxanone"
1894 Methyl-*3*-oxobutanoate
37 Methyl-(*1*-oxy-cyclohexyl)-ketone
1879 Methyl-*2*-oxy-*4*-methoxybenzoate
2155 .... Methyl-*2*-oxy-*5*-methoxybenzoate
165 "Methyl patchone"
2127 Methyl-*gamma*-pelargolactone
2128 Methyl pelargonate
2970 *para*-Methyl pelargophenone
2156 *2*-Methyl-*2*,*4*-pentanediol
2156 .... *5*-Methyl-*1*,*3*-pentanediol
32 *4*-Methyl-*2*,*3*-pentanedione
2263 Methylpentanoate
2264 Methyl-*iso*-pentanoate
2265 *2*-Menthylpentan-*1*-oic acid
2267 *2*-Menthylpentan-*5*-oic acid
2266 *3*-Methylpentan-*1*-oic acid
2267 *4*-Methylpentan-*1*-oic acid
2157 .... *d*-*3*-Methylpentanol-*1*
1925 *4*-Methyl-*2*-pentanol
2014 *3*-Methylpentan-*2*-one
1933 *4*-Methyl-*2*-pentanone
1637 *2*-Methylpentan-*5*-yl acetate
1647 *2*-Methylpentan-*5*-yl-*n*-butyrate
954 *3*-Methyl-*2*-(*n*-pentanyl)-cyclopenten-*2*-one-*1*
1686 *2*-Methylpentan-*5*-yl-*beta*-methylbutyrate
2015 *2*-Methyl-*2*-pentenal
1304 *2*-Methylpentenoic acid, ethylester
2158 .... *3*-Methyl-*3*-penten-*1*-ol
1605 *4*-Methyl-*3*-penten-*1*-ol
1856 *4*-Methyl-*3*-penten-*2*-one
2159 .... Methyl pentenyl acetate

1610 *4*-Methyl-*3*-penten-*1*-yl acetate
2160 .... Methyl pentenyl benzoate
2161 .... Methyl pentenyl-*iso*-butyrate
1904 Methyl-*4*-pentenyl carbinol
2162 .... *4*-(*4*-Methyl-*3*-penten-*1*-yl)-*3*-cyclohexene-*1*-carboxaldehyde
1788 *3*-Methyl-*2*-(*cis*-*3*-penten-*1*-yl)-*2*-cyclopenten-*1*-one
1790 *3*-Methyl-*2*-(*trans*-*2*-pentenyl)-*2*-cyclopenten-*1*-one
2163 .... Methyl pentenyl formate
472 Methyl pentenyl ketone
2164 .... Methyl pentenyl phenylacetate
2165 .... Methyl pentenyl propionate
2166 .... Methyl pentenyl salicylate
2107 Methyl pentin carbonate
2167 .... Methyl-*n*-pentin carbonate
2908 *3*-Methyl-*2*-(*n*-pentyl)-cyclopentanone-*1*
954 Methyl-*3*-pentyl-*2*-cyclopenten-*2*-one-*1*
2156 Methyl-*beta*-pentyleneglycol
2167 Methyl pentyne carbonate
2168 .... *N*-Methyl phenethyl carbamide
2192 Methyl phenethyl ether
707 *meta*-Methyl phenol
708 *para*-Methyl phenol
1696 *alpha*-Methyl phenylacetaldehyde
2954 *para*-Methyl phenylacetaldehyde
2169 .... Methyl phenylacetate
1691 *alpha*-Methyl-*gamma*-phenylallyl alcohol
2200 *3*-Methyl-*5*-phenyl-*n*-amylalcohol
2965 *ortho*-Methyl-*2*-phenyl-(*1*,*3*-benzthiazole)
2170 .... *2*-Methyl phenyl benzylether
2170 Methyl phenyl benzyl oxide
2172 *alpha*-Methyl-*gamma*-phenylbutanal
2016 *2*-Methyl-*1*-phenylbutan-*2*-ol
2670 *3*-Methyl-*1*-phenyl-*2*-butanol
2228 *3*-Methyl-*2*-phenyl-*2*-butanol
1916 *1*-Methyl-*1*-phenylbutanone-*3*
3061 *3*-Methyl-*1*-phenyl-*1*-butanone
1916 *4*-Methyl-*4*-phenyl-*2*-butanone
1044 *2*-Methyl-*4*-phenylbutan-*2*-yl acetate
513 *2*-Methyl-*4*-phenylbutan-*4*-yl acetate
1046 *2*-Methyl-*4*-phenylbutan-*2*-yl-*iso*-butyrate
2171 .... *3*-Methyl-*4*-phenyl-*3*-buten-*2*-one
2172 .... *2*-Methyl-*4*-phenyl butyraldehyde
2173 .... *3*-Methyl-*2*-phenyl butyraldehyde
2174 .... Methyl phenylbutyrate
2175 .... Methyl phenyl carbinol
2176 .... Methyl phenyl carbinyl acetate
2177 .... Methyl phenyl carbinyl anthranilate
2178 .... Methyl phenyl carbinyl benzoate
2179 .... Methyl phenyl carbinyl-*n*-butyrate
2180 .... Methyl phenyl carbinyl-*iso*-butyrate
2181 .... Methyl phenyl carbinyl caproate
2182 .... Methyl phenyl carbinyl caprylate
2183 .... Methyl phenyl carbinyl cinnamate
2184 .... Methyl phenyl carbinyl formate
2182 Methyl phenyl carbinyl octoate
2185 .... Methyl phenyl carbinyl phenylacetate
2186 .... Methyl phenyl carbinyl propionate
2187 .... Methyl phenyl carbinyl salicylate
2185 Methyl phenyl carbinyl-*alpha*-toluate
2188 .... Methyl phenyl carbinyl-*iso*-valerate
2074 *2*-Methyl-*3*-phenyl-*1*,*1*-dimethoxy-propane
11 *2*-Methyl-*4*-phenyl-*1*,*3*-dioxolane
274 *4*-Methyl-*2*-phenyl-*meta*-dioxolane
246 Methyl phenyl ether
1705 *alpha*-Methyl phenylethyl acetate
1918 *alpha*-Methyl-*beta*-phenylethyl acetate
2189 .... *para*-Methyl phenylethyl acetate
1707 *alpha*-Methyl phenylethyl alcohol
1917 *alpha*-Methyl-*beta*-phenylethyl alcohol
2190 *aryl*-Methyl phenylethyl alcohol
2190 .... *ortho*-Methyl phenylethyl alcohol
2191 .... *para*-Methyl phenylethyl alcohol
2538 Methyl phenylethyl carbinol
2539 Methyl phenylethyl carbinyl acetate
2540 Methyl phenylethyl carbinyl-*iso*-valerate
2192 .... Methyl phenylethyl ether
288 Methyl phenylethyl ketone
2168 Methyl phenylethyl urea
2193 .... Methyl phenyl glycidate
1306 Methyl phenyl glycidic acid, ethylester
2117 Methyl phenyl glycidic acid, methylester
2194 .... *2*-Methyl-*2*-phenyl hexanone-*4*
24 Methyl phenyl ketone
2248 *5*-(*3*-Methylphenyl)-*2*-methyl amyl alcohol
2247 *para*-Methylphenyl methyl carbinol
2195 .... Methyl phenyl nonyl carbinol
2204 Methyl phenyl pentanal
2196 .... *2*-Methyl-*5*-phenylpentanol-*1*
2197 .... *2*-Methyl-*5*-phenylpentanol-*2*
2198 .... *2*-Methyl-*5*-phenylpentanol-*3*
2199 .... *2*-Methyl-*2*-phenylpentanol-*4* (see also 2576)
2200 .... *3*-Methyl-*5*-phenylpentanol-*1*
2541 *3*-Methyl-*1*-phenylpentanol-*3*
407 *4*-Methyl-*1*-phenylpentanol-*2*
2201 .... *4*-Methyl-*1*-phenyl-*2*-pentanone
1706 *5*-Methyl-*5*-phenyl pentanone
2072 *2*-Methyl-*3*-phenyl propanal
405 *2*-Methyl-*2*-phenyl propane
2021 *1*-Methyl-*1*-phenyl propanol-*1*
2071 *2*-Methyl-*3*-phenylpropanol-*1*
2502 *3*-Methyl-*3*-phenylpropanol-*1*
3100 *3*-(*3'*-Methylphenyl)-propanol-*1*
1951 *2*-Methyl-*3*-phenyl-*2*-propenal
1951 *3*-Methyl-*3*-phenyl-*2*-propenal
1949 Methyl-*3*-phenylpropenoate
1950 *alpha*-Methyl-*3*-phenyl-*2*-propen-*1*-ol
1954 *2*-Methyl-*3*-phenyl-*2*-propen-*1*-yl acetate
2202 .... Methyl phenyl propionate
2070 *2*-(*para*-Methylphenyl)-propionic aldehyde
2072 *2*-Methyl-*3*-phenylpropionic aldehyde
2073 *4*-Methyl phenylpropionic aldehyde
2022 *1*-Methyl-*1*-phenylpropyl acetate

2075 *2*-(*alpha*)-Methyl-*3*-phenylpropyl acetate
2196 *beta*-Methyl-*beta*-phenylpropyl ethanol
2203 .... Methyl phenylpropyl ether
328 Methyl phenylpropyl ketone
1126 *beta*-Methyl phenyl styryl ketone
2204 .... *3*-Methyl-*4*-phenyl valeric aldehyde
1051 Methyl phthalate
2205 .... Methyl piperonylate
2010 Methyl piperonyl ketone
548 *2*-Methylpropanal
2209 Methyl propanoate
550 *2*-Methyl propanoic acid
390 *2*-Methyl-*1*-propanol
392 *2*-Methylpropanol-*2*
1857 *2*-Methyl propenal
2206 .... Methyl-*2*-*iso*-propenyl-*5*-anisole
2206 *2*-Methyl-*5*-*iso*-propenyl-*5*-anisole
2207 .... *1*-Methyl-*4*-*iso*-propenyl benzene
1859 *2*-Methylpropenyl-*n*-butyrate
2878 *1*-Methyl-*4*-*iso*-propenyl cyclohexan-*1*-ol
2768 *1*-Methyl-*4*-*iso*-propenyl cyclohexan-*3*-ol
926 *6*-Methyl-*3*-*iso*-propenyl cyclohexanol
927 *1*-Methyl-*4*-*iso*-propenylcyclohexanone-*2* acetate
2770 *1*-Methyl-*4*-*iso*-propenyl-*3*-cyclohexanone
2771 *1*-Methyl-*4*-*iso*-propenylcyclohexan-*3*-yl acetate
928 *6*-Methyl-*3*-*iso*-propenyl cyclohexanyl acetate
1800 *1*-Methyl-*para*-*iso*-propenyl-*1*-cyclohexene
2870 *1*-Methyl-*3*-*iso*-propenyl-*1*-(or -*6*-)-cyclohexene
1074 *1*-Methyl-*4*-*iso*-propenyl-*1*-cyclohexene
578 *1*-Methyl-*4*-*iso*-propenyl cyclohexen-*6*-ol-*2*
2629 *1*-Methyl-*4*-*iso*-propenyl-*1*-cyclohexen-*3*-one
579 *d*-*1*-Methyl-*4*-*iso*-propenyl-*6*-cyclohexen-*2*-one
580 *l*-*1*-Methyl-*4*-*iso*-propenyl-*6*-cyclohexen-*2*-one
2456 *4*-(*2*-Methyl-*5*-*iso*-propenyl-*1*-cyclopentenyl)-*2*-butanone
1860 *2*-Methyl propenyl hexoate
2809 *cis*-*2*-(*2*′-Methyl-*1*′-propenyl)-*4*-methyl tetrahydropyran
2208 .... *1*-Methyl-*2*-propenyl-*4*-*iso*-propylbenzene
2209 .... Methyl propionate
2210 .... Methyl-*N*-propionyl anthranilate
723 *1*-Methyl-*4*-propoxybenzene
2265 Methyl propyl acetic acid
2211 .... Methyl-*iso*-propyl acetophenone
2212 .... *5*-Methyl-*2*-*iso*-propyl-*1*-acetyl-*5*-cyclohexene
574 *2*-Methyl-*5*-*iso*-propyl acetyl phenol
2053 Methyl-*beta*-propyl acrylate
2751 *1*-Methyl-*4*-*n*-propyl aminobenzene
819 *para*-Methyl-*iso*-propylbenzene
575 *2*-Methyl-*5*-*iso*-propyl benzoyl phenol
2228 Methyl-*iso*-propyl benzyl alcohol
3021 *4*-Methyl-*1*-*iso*-propyl-bicyclo-(*0* : *1* : *3*)-hexen-*3*-one-*2*
127 Methyl-*n*-propyl carbinol
139 Methyl-*n*-propyl carbinyl butyrate
2213 .... *alpha*-Methyl-*para*-*iso*-propyl cinnamic aldehyde
2873 *1*-Methyl-*4*-*iso*-propylcyclohexadiene-*1*,*3*
2874 *1*-Methyl-*4*-*iso*-propyl-*1*,*4*-cyclohexadiene
2459 *2*-Methyl-*5*-*iso*-propyl-*1*,*3*-cyclohexadiene
1836 *1*-Methyl-*4*-*iso*-propyl cyclohexane
2880 *1*-Methyl-*4*-*iso*-propyl cyclohexanediol-*1*,*8*-hydrate
2313 *1*-Methyl-*4*-*iso*-propyl cyclohexan-*3*-ol
970 *1*-Methyl-*4*-*iso*-propyl cyclohexanol-*8*
1840 *5*-Methyl-*2*-*iso*-propyl cyclohexanol
265 *1*-Methyl-*4*-*iso*-propylcyclohexene-*2*-dioxide-*1*,*4*
2876 *1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*4*-ol
2875 Methyl-*4*-*iso*-propyl-*3*-cyclohexen-*1*-ol
2877 *1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*8*-ol
1069 *1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*2*-ol-*3*-one
2630 *1*-Methyl-*4*-*iso*-propyl-*1*-cyclohexen-*3*-one
2214 .... *1*-Methyl-*4*-propyl-*1*-cyclohexenone-*5*
2215 *1*-Methyl-*5*-*n*-propyl-*1*-cyclohexen-*3*-one
581 *3*-Methyl-*4*-*iso*-propylcyclohexen-*6*-one-*2*
2215 .... *3*-Methyl-*5*-propyl-*2*-cyclohexenone
2214 *3*-Methyl-*6*-propyl-*3*-cyclohexenone
2212 *5*-Methyl-*2*-*iso*-propyl-*5*-cyclohexenyl methyl ketone
2219 *1*-(*1*-Methyl-*1*-(*4*-*iso*-propylcyclohexyl))-*1*-propanone
2216 .... *3*-Methyl-*4*(*4*′-*iso*-propylcyclohexyl)-butanol
2217 .... *3*-Methyl-*4*(*4*′-*iso*-propylcyclohexyl)-butan-*2*-one
31 Methyl propyl diketone
32 Methyl-*iso*-propyl diketone
2218 .... Methyl-*1*-propyl disulfide
453 Methyl-*iso*-propyl formate
577 *2*-Methyl-*5*-*iso*-propyl formyl phenol
1840 *5*-Methyl-*2*-*iso*-propyl hexahydrophenol
2219 .... *alpha*-Methyl-*para*-*iso*-propyl hexahydro phenylethyl ketone
2909 *5*-Methyl-*2*-*iso*-propylhexanol-*1*
2910 *5*-Methyl-*2*-*iso*-propylhexan-*1*-yl acetate
2911 *5*-Methyl-*2*-*iso*-propylhexan-*1*-yl-*n*-butanoate
2912 *5*-Methyl-*2*-*iso*-propylhexan-*1*-yl-*iso*-butanoate
959 *5*-Methyl-*2*-*iso*-propyl-*4*-hexen-*1*-al

957 *2*-Methyl-*6*-*iso*-propyl-*4*-hexenol
2220 .... *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamic alcohol
758 *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamic aldehyde
2221 .... *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamic aldehyde ethyleneglycol acetal
2222 .... *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamic aldehyde monomethyl acetal
2223 .... *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamyl acetate
2224 .... *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamyl butyrate
2225 .... *alpha*-Methyl-*para*-*iso*-propyl hydrocinnamyl propionate
2942 *2*-Methyl-*5*-*iso*-propyl hydroquinone
2879 *1*-Methyl-*4*-*iso*-propylidene cyclohexanol-*1*
2767 *1*-Methyl-*4*-*iso*-propylidene cyclohexanol-*3*
2769 *1*-Methyl-*4*-*iso*-propylidene-*3*-cyclohexanone
2628 *1*-Methyl-*4*-*iso*-propylidene-*1*-cyclohexen-*3*-one
959 *5*-Methyl-*2*-*iso*-propylidene hexanal-*1*
957 *5*-Methyl-*2*-*iso*-propylidene-*1*-hexanol
2226 .... Methyl propyl ketone
2227 .... Methyl-*iso*-propyl ketone
1052 *1*-Methyl-*7*-*iso*-propyl naphthalene
2945 *2*-Methyl-*4*-*iso*-propylphenol
573 *2*-Methyl-*5*-*iso*-propylphenol
2945 *2*-Methyl-*6*-*iso*-propylphenol
2945 *3*-Methyl-*2*-*iso*-propylphenol
2945 *3*-Methyl-*4*-*iso*-propylphenol
2945 *3*-Methyl-*5*-*iso*-propylphenol
2944 *3*-Methyl-*6*-*iso*-propylphenol
2944 *5*-Methyl-*2*-*iso*-propylphenol
2945 *6*-Methyl-*3*-*iso*-propylphenol (see also 573)
2228 .... Methyl-*iso*-propyl phenylcarbinol
17 Methyl-(*4*-*iso*-propylphenyl)-ketone
759 Methyl-*N*-(*3*-(*para*-*iso*-propylphenyl)-*2*-methylpropylidene)-anthranilate
1932 *2*-Methyl-*3*-*para*-*iso*-propylphenyl-*1*-propanal
758 *alpha*-Methyl-*para*-*iso*-propyl phenylpropionaldehyde
2948 *3*-Methyl-*6*-*iso*-propyl phenylpropionate
2942 *2*-Methyl-*5*-*iso*-propyl quinol
2229 .... Methyl-*1*-propyl trisulfide
3077 "Methyl protechin"
3067 Methyl protocatechuic aldehyde
46 Methyl-*3*-pyridyl ketone
1831 *3*-Methyl pyromeconic acid
2033 Methyl pyromucate
2230 .... *5*-Methyl-*alpha*-pyrone
2230 *5*-Methyl-*2*-pyrone
2231 .... *1*-Methyl pyrrole
2232 .... Methyl pyrrolidine
2233 .... Methyl quinoline (summary of Methyl quinolines)
2234 .... *alpha*-Methyl quinoline
2233 *ana*-Methylquinoline
2233 *beta*-Methylquinoline
2235 *gamma*-Methylquinoline
2234 *2*-Methylquinoline
2233 *3*-Methylquinoline
2235 .... *4*-Methyl quinoline
1948 *4*-Methyl-*alpha*-quinoline
2233 *5*-Methylquinoline
2236 .... *meta*-Methyl quinoline
2237 .... *ortho*-Methyl quinoline
2238 .... *para*-Methyl quinoline
2238 *6*-Methylquinoline
2236 *7*-Methylquinoline
2237 *8*-Methylquinoline
1948 *4*-(or *gamma*-)-Methyl-*2*-quinolinol
2441 *5*-Methylresorcinol dimethylether
2442 *5*-Methylresorcinol monomethylether
2239 .... Methyl ricinoleate
2240 .... *4*-Methyl safranal
1864 Methyl salicylaldehyde
2241 .... Methyl salicylate
2012 Methyl salicylate, ethylether
1877 Methyl salicylate, methylether
1865 *2*-Methylsaligenin acetate
1058 Methyl sebacate
1026 "Methyl skatole"
2242 .... Methyl stearate
1691 Methyl styryl carbinol
318 Methyl styryl ketone
1059 Methyl succinate
1060 Methyl sulfide
2121 Methyl tetradecanoate
2928 *4*-Methyl-*1*,*2*,*5*,*6*-tetrahydro benzaldehyde
1975 *6*-Methyl tetrahydrobenzylidene methyl ethyl ketone
1716 *alpha*-Methyl tetrahydroquinoline
2917 *para*-Methyl tetrahydroquinoline
558 Methyl theobromine
2243 .... *4*-Methyl thiazolyl ethanol-*5*
2100 Methyl thiobutanal
2120 *beta*-Methyl thiolpropionic acid, methylester
2245 *3*-Methyl thiol propylalcohol
2952 *beta*-Methyl thiophene
2244 *3*-Methyl thiopropanal
2245 *3*-Methyl thiopropanol
2244 .... *3*-Methyl thiopropionaldehyde
2245 .... *3*-Methyl thiopropyl alcohol
1696 *alpha*-Methyl tolualdehyde
2169 Methyl-*alpha*-toluate
2246 .... Methyl-*para*-toluate
2578 *alpha*-Methyl-*alpha*-toluic acid
2247 .... Methyl-*para*-tolyl carbinol
1921 *5*-Methyl-*2*-*meta*-tolyl-*1*,*3*-dioxolane
717 Methyl-*meta*-tolylether
718 Methyl-*ortho*-tolylether
719 Methyl-*para*-tolylether
1895 Methyl-*para*-tolyl ketone
2248 .... *2*-Methyl-*5*-*meta*-tolyl pentanol
2249 .... *2*-Methyl-*3*-tolyl propionaldehyde
1377 *2*-Methyl-*4*-(*1*,*1*,*3*-trimethyl-*2*′-cyclohexen-*2*′-yl)-butadiene methylketone

2250 .... *2*-Methyl-*4*-(*2,6,6*-trimethyl-*1*-(or -*2*-) cyclohexenyl)-*3*-buten-*1*-al
2251 *3*-Methyl-*4*-(*2,3,5*-trimethyl-*4*-cyclohexenyl)-*3*-buten-*2*-one
2251 .... *3*-Methyl-*4*-(*2,4,6*-trimethyl-*3*-cyclohexenyl)-*3*-buten-*2*-one
1377 *4*-Methyl-*6*-(*1,1,3*-trimethyl-*2'*-cyclohexen-*2'*-yl)-*3,5*-hexadien-*2*-one
2252 .... Methyl-*3,5,6*-trimethyl-*3*-cyclohexenyl ketone
2253 .... Methyl-*N*-(*3,5,5*-trimethylhexylidene)-anthranilate
2254 .... Methyl trisulfide
2255 .... Methyl umbelliferone
2013 *beta*-Methylumbelliferone ethylether
2256 .... Methyl umbelliferone methylether
2132 *2*-Methylundecanal
2257 .... Methyl undecanoate
2258 .... *2*-Methyl undecanol
2258 *3*-Methylundecanol-*3*
2258 *6*-Methylundecanol
2259 .... Methyl-*9*-undecenoate
2260 .... Methyl-*n*-undecin carbonate
2261 .... Methyl undecyl acetaldehyde
2257 Methyl undecylate
2259 Methyl undecylenate
2262 .... Methyl undecyl ketone
2260 Methyl-*n*-undecyne carboxylate
1996 Methyl-*2*-undecynoate
2263 .... Methyl valerate
2108 Methyl-*active*-valerate
2264 .... Methyl-*iso*-valerate
2263 Methyl valerianate
2264 Methyl-*iso*-valerianate
2265 *alpha*-Methylvaleric acid
2266 *beta*-Methylvaleric acid
2265 .... *2*-Methyl valeric acid
2266 .... *3*-Methyl valeric acid
2267 .... *4*-Methyl valeric acid
2264 *3*-Methyl-*2*-*iso*-valeroyl furan
3077 Methyl vanillin
567 *8*-Methyl-*N*-vanillyl-*6*-nonenamide
2649 "Methyl vanitrope"
2268 .... *gamma*-Methyl-*gamma*-vinyl butyrolactone
376 *2*-(Methylvinyl carbinyl)-cyclopentan-*1*-ol
2316 Methyl vinyl homogeranyl carbinol
1804 *2*-Methyl-*2*-vinyl-*5*-hydroxy-*iso*-propyl tetrahydrofuran
2269 .... Methyl vinyl ketone
2270 .... *7*-Methyl-*3*-vinyl-*6*-octen-*1*-ol
2809 *3*-Methyl-*4*-vinyl-*6*-*iso*-propenyl tetrahydropyran (see also 3016)
2809 *2*-Methyl-*4*-vinyl-*5*-*iso*-propylidene tetrahydropyran (see also 3016)
982 "Methylzingerone"
2045 M.H.C.
2854 "Micromet"
1207 "Mignonette"
1793 Milk sugar
1051 Mipax
2332 Mirbane oil
2132 M.N.A.
2140 M.N.K.
2145 M.O.A.
2271 .... Monoacetin
2271 *1*-Monoacetin
2271 *2*-Monoacetin
2273 Monoammonium glutamate
1141 Monoethyl aconitate
1221 Monoethylglycol
1222 Monomethyl glycol
1722 "Monomethyl hydroquinone"
2442 "Monomethyl orcin"
3068 *para*-Monomethyl protocatechualdehyde
2272 .... Mononitro dibromobutyl-*meta*-cresol methylether
1469 Mono olein
2273 Monopotassium glutamate
2563 Mono phenylethylene glycol
1223 Monophenyl glycol
1224 Monopropyl glycol
2273 .... Monosodium glutamate
2274 .... Monosodium-*l*-homocysteinate
1470 *alpha*-Monostearin
306 "Morellone"
1062 "Moscatol"
2275 .... Moskene
105 "Moskus lakton"
2858 Mountain Ash (see also 2714)
2246 M.p.T.
2273 "M.S.G."
1731 "Muguene"
688 "Muguet aldehyde" (see also 697)
2566 "Muguet Principe"
1728 "Muguet synthétique"
1728 "Muguettine Principe"
1030 Muguol
2443 "Musc 906"
3017 "Musc Baur"
1985 "Muscenone"
811 "Muscolacton"
811 "Muscolide"
2276 .... Muscone
1982 "*iso*-Muscone"
2277 .... Muscopyridine
813 "Muscosyn"
3080 "Musk 36 A"
1066 "Musk aldehyde"
2278 .... Musk ambrette
1067 "Musk cyanide"
2279 .... Musk ketone
2280 .... Musk ketone – methylanthranilate
2444 "Musk R.1."
1214 "Musk T."
2281 .... Musk tibetene
3017 "Musk Toluene"
2282 "Musk Xylene"
2282 .... Musk xylol
98 Mustard oil, artificial
2162 "Myrac aldehyde"
2283 .... Myrcene
2284 .... Myrcenol
2285 .... Myrcenyl acetate (see also 2763)
2286 .... Myrcenyl formate
2287 .... Myrcenyl propionate
2290 Myristaldehyde
2288 .... Myristic acid

2289 .... Myristic alcohol
2290 .... Myristic aldehyde
2291 .... Myristicin
2292 .... Myristic nitrile
2289 Myristyl alcohol
2293 .... Myrtenal
2294 .... Myrtenol
2295 .... Myrtenyl acetate
2294 Myrtol

N
789 "Nadone" (see also 777)
2365 "N.A.ester"
2296 .... Naphthalene
2296 Naphthene
2297 .... *beta*-Naphthol benzylether
2298 .... *beta*-Naphthol-*n*-butylether
2299 .... *beta*-Naphthol-*iso*-butylether
2300 .... *beta*-Naphthol-*secondary*-butylether
2301 .... *beta*-Naphthol ethylether
2302 .... *beta*-Naphthol methylether
2303 .... *beta*-Naphthol phenylether
2304 .... *beta*-Naphthol propylether
2305 .... *alpha-1,4*-Naphthoquinone
2306 *2*-Naphthyl-*ortho*-aminobenzoate
2306 .... *beta*-Naphthyl anthranilate
2307 *beta-1*-Naphthyl ethanol
2307 .... *beta*-Naphthyl ethylalcohol
2308 .... *beta*-Naphthyl formate
2308 *2*-Naphthyl methanoate
2124 *beta*-Naphthyl methylketone
2577 Naphthyl phenylketone
2122 *2-beta*-Naphthyl propionaldehyde
725 "Narceol" (see also 739)
739 "Narcissin"
730 "Narcissin K"
2309 .... Naringin
2310 .... Naringin dihydrochalcone
2850 "Natron"
913 "Neantine"
529 "Nefolia"
2763 "Neobergamate"
2139 "Neofolione"
2311 .... Neohesperidin dihydrochalcone
2312 .... Neo-irone (summary of Neo-irones)
2313 .... *dextro*-Neomenthol (see also 1839)
1841 *dl*-Neomenthol
122 Neopentyl acetate
2314 .... Nepetalactone
649 Neral
2315 Neraniol
2315 Nerodol
2315 Nerogenol
2315 .... Nerol
2316 .... Nerolidol
2317 .... Nerolidyl acetate
2318 .... Nerolidyl-*iso*-butyrate
2319 .... Nerolidyl formate
2320 .... Nerolidyl propionate
2302 Nerolin I
2301 Nerolin II
2301 Nerolin "Bromelia"
2299 Nerolin "Fragarol"
2302 Nerolin "Yara-Yara"
2315 Nerolol
2124 Nerolon
2123 "Nerolys" (see also 2124)
2321 .... Nerone
2315 Nerosol
2322 .... Neryl acetate
2323 .... Neryl benzoate
2324 .... Neryl butyrate
2324 Neryl-*n*-butyrate
2325 .... Neryl-*iso*-butyrate
2326 .... Neryl caproate
2327 .... Neryl formate
2326 Neryl hexanoate
2326 Neryl hexoate
2326 Neryl hexylate
2331 Neryl-*beta*-methylbutyrate
2330 Neryl pentanoate
2328 .... Neryl phenylacetate
2329 .... Neryl propionate
2328 Neryl-*alpha*-toluate
2330 .... Neryl valerate
2331 .... Neryl-*iso*-valerate
2330 Neryl-*n*-valerianate
2331 Neryl-*iso*-valerianate
351 Ngai camphor
1912 Niobe oil (see also 1159)
2718 Nipasol
1311 Nitric ether, alcoholic solution
112 *4*-Nitro-*2*-aminophenyl allylether
112 *4*-Nitro-*2*-aminophenyl-*n*-butylether
112 *4*-Nitro-*2*-aminophenyl ethylether
112 *4*-Nitro-*2*-aminophenyl methylether
112 *4*-Nitro-*2*-aminophenyl propylether
112 *4*-Nitro-*2*-aminophenyl-*iso*-propylether
2332 .... Nitrobenzene
2332 Nitrobenzol
2333 .... Nitrocumene
2334 .... Nitrocyclohexane
2272 *2*-Nitro-*3,5*-dibromo-*4-tertiary*-butylanisole
2335 .... *para*-Nitrophenol
2336 .... *1*-Nitro-*2*-phenylethane
2337 "*para*-Nitrophenyl mustard oil"
2333 *2*-Nitro-*2*-phenylpropane
2337 .... *4*-Nitrophenyl-*iso*-thiocyanate
2333 *alpha*-Nitro-*iso*-propylbenzene
2338 .... *ortho*-Nitrotoluene
1311 Nitrous and Nitric ethers, alcoholic solution
558 "No-Doz"
2796 "Noisettal"
1719 "Noisette"
2339 .... Nonadienal
2340 .... Nonadienal diethyl acetal
2341 .... Nonadienol
2342 .... *delta*-Nonalactone
2350 *gamma*-Nonalactone
2348 "Nonalol"
2343 .... *n*-Nonanal
2344 .... Nonanal diethyl acetal
2345 .... Nonanal dimethyl acetal
840 Nonanecarbonic acid-*1*
2346 "Nonane diacetate"
2346 .... Nonanediol-*1:2*-acetate
2346 Nonane diol monoacetate
2347 .... Nonanoic acid

2343 Nonanoic aldehyde
2348 .... Nonanol-*1*
2048 *2*-Nonanol
2349 .... *3*-Nonanol
2363 Nonanol acetate
2354 *3*-Nonanol acetate (see also 2364)
2374 Nonanol formate
2371 Nonanol hexanoate
2375 Nonanol heptylate
2350 .... Nonanolide-*1 : 4*
2342 Nonanolide-*1 : 5*
140 "*iso*-Nonanolide" (see also 2142)
2376 Nonanol-*alpha*-methylacrylate
2376 Nonanol-*2*-methylpropenoate
2377 Nonanol nonanoate
2372 Nonanol octanoate
2379 *n*-Nonanol-*n*-pentanoate
2380 Nonanol-*iso*-pentanoate
2378 *n*-Nonanol propanoate
2052 *2*-Nonanone
2351 .... *3*-Nonanone
886 Nonanone-*5*
480 *iso*-Nonanone
2352 .... *3*-Nonanon-*1*-yl acetate
2353 *N*-Nonanoyl-*4*-hydroxy-*3*-methoxybenzene
2355 Nonanoyl piperidine
2353 .... Nonanoyl vanillylamide
2354 .... Nonanyl acetate
2355 .... Nonanyl piperidine
200 Nonate
1579 *3,5,7*-Nonatrien-*2*-one
356 .... *2*-Nonenal
1252 "*iso*-Nonenoic aldehyde"
2362 *2*-Nonenoic nitrile
57 .... *omega*-Nonenol
1687 Nonen-*1*-ol-*3*
1687 *3*-Nonen-*1*-ol
2050 *2*-Nonenol-*7*
2357 *8*-Nonen-*1*-ol
58 .... Nonen-*5*-one-*2*
59 .... *3*-Nonenyl acetate
1101 Nonenyl acrolein
2357 *omega*-Nonenyl alcohol
2356 *alpha*-Nonenyl aldehyde
0 .... *alpha*-Nonenyl cinnamic aldehyde
2130 *iso*-Nonenyl cyanide
1 .... *alpha*-Nonenyl furfuracrolein
2361 *alpha*-Nonenyl-*beta*-*2*-furylacrolein
2361 *alpha*-Nonenyl-*3*-(*2*-furyl)-propenal
2 .... Nonenyl nitrile
2381 Noninol acetate
2347 Nonoic acid
2343 Nonoic aldehyde
3 .... Nonyl acetate
3008 "*iso*-Nonyl acetate"
1 .... *secondary*-Nonyl acetate
1110 *3*-Nonyl acrolein
2348 Nonyl alcohol
3007 "*iso*-Nonylalcohol"
2343 *n*-Nonylaldehyde
2056 "*iso*-Nonylaldehyde" (see also 3006)
2344 *n*-Nonylaldehyde diethyl acetal
2345 *n*-Nonylaldehyde dimethyl acetal
2253 "*iso*-Nonylaldehyde"-methylanthranilate
1111 *3*-Nonyl allylalcohol
2365 *n*-Nonyl-*ortho*-aminobenzoate
2365 .... Nonyl anthranilate
2366 .... Nonyl benzoate
2367 Nonyl butanoate
2368 *n*-Nonyl-*iso*-butanoate
2367 .... Nonyl-*n*-butyrate
2368 .... Nonyl-*iso*-butyrate
2369 .... *alpha-n*-Nonyl butyrolactone
2370 .... *gamma-n*-Nonyl-*gamma*-butyrolactone
2371 .... *n*-Nonyl caproate
2372 .... Nonyl caprylate
841 Nonyl carbinol
2360 *alpha-n*-Nonyl cinnamic aldehyde
2373 .... *para*-Nonyl cyclohexanone
2050 "*iso*-Nonylene alcohol"
2356 *alpha-beta*-Nonylene aldehyde
2363 *n*-Nonyl ethanoate
2374 .... Nonyl formate
2375 *n*-Nonyl heptanoate
2375 .... Nonyl heptoate
2375 Nonyl heptylate
1554 Nonyl heptylether
2371 Nonyl hexoate
2371 Nonyl hexylate
2347 *n*-Nonylic acid
2350 *gamma*-Nonyllactone
2376 .... Nonyl methacrylate
2374 *n*-Nonyl methanoate
2140 Nonyl methyl ketone
2195 Nonyl methyl phenyl carbinol
2377 *n*-Nonyl-*n*-nonylate
2372 Nonyl octoate
2372 *n*-Nonyl octylate
2377 .... Nonyl pelargonate
2378 .... Nonyl propionate
2379 .... Nonyl-*n*-valerate
2380 .... Nonyl-*iso*-valerate
2380 Nonyl-*iso*-valerianate
2448 *2*-Nonyn-*1*-al dimethylacetal
2381 .... Nonynol acetate
2381 *2*-Nonyn-*3*-ol acetate
2382 Nootkatin
2382 .... Nootkatone
2620 Nopinene
2383 .... Nopol
2384 .... Nopyl acetate
2385 .... Nopyl-*n*-butyrate
2386 .... Nopyl propionate
2387 .... Nor-bornadiene
942 Nor-borneol
817 Nor-bornenyl acetate
943 Nor-bornyl acetate
818 Nor-bornylenyl ethylcarbonate
817 Nor-camphenyl acetate
818 Nor-camphenyl ethylcarbonate
2834 *π*-Nor-camphor
3015 Nor-hexahydro farnesal
168 "Nor-*iso*-jasmone"
810 Nor-muscol
813 Nor-muscone
3014 Nor-tetrahydrofarnesal

3013 Nor-tetrahydrofarnesol
13 Novatone
2086 Noviraldiol
1363 Novovanillin
13 Nyobepine

**O**

2388 .... Ocimene (see also 59)
2389 .... Ocimenol
2390 .... *cis*-Ocimenyl acetate
2813 Ocotea oil
2868 Octa-acetyl sucrose
2391 .... Octadecanal
2863 Octadecanoic acid
2392 .... Octadecanol-*1*
2440 *9*-Octadecenoic acid
2392 *n*-Octadecyl alcohol
2393 .... Octadienal
2394 .... Octadienol
1791 Octahydro-*3*,*5*,*5*-*8*,*8*-pentamethyl-*3*-(*1*-*H*)-naphthalenone
416 Octalactone
2403 *gamma*-*n*-Octalactone
2395 .... *gamma*-*iso*-Octalactone
2397 *n*-Octaldehyde
2396 Octamethylene carbonate
2396 .... Octamethylene carboxylate
2397 .... *n*-Octanal
2397 Octanal-*1*
2398 .... Octanal diethyl acetal
2399 .... Octanal dimethyl acetal
2347 Octane-*1*-carboxylic acid
2837 Octane-*1*,*8*-dicarboxylic acid
1058 *1*,*8*-Octanedicarboxylic acid, dimethylester
33 *2*,*3*-Octane dione
891 *4*,*5*-Octane dione
2400 .... Octanoic acid
2040 *iso*-Octanoic acid
2401 .... Octanol-*1*
2402 *d*-*n*-Octanol
2057 *2*-Octanol
2402 .... *3*-Octanol
2403 .... Octanolide-*1* : *4*
2395 *iso*-Octanolide-*1* : *4*
1757 *5*-Octanol-*4*-one
2066 *2*-Octanone
1148 *3*-Octanone
2404 .... *3*-Octanon-*1*-ol
2408 Octanyl acetate
2405 .... *2*-Octanyl acetate
2406 .... *3*-Octanyl acetate
1265 *3*-Octanyl acrylate
2413 *2*-Octanyl-*iso*-butyrate
2413 *3*-Octanyl-*iso*-butyrate
2059 *2*-Octanyl formate
2059 *3*-Octanyl formate
2434 *2*-Octanyl phenylacetate
2434 *3*-Octanyl phenylacetate
124 *2*-Octenal
2421 *1*-Octene
2407 .... *2*-Octenoic acid
231 *1*-Octen-*3*-ol
231 *3*-Octenol
232 *1*-Octen-*3*-yl acetate
2044 "*2*-Octenyl acetate"
232 *beta*-Octenyl acetate
3022 Octenyl acrolein
233 *1*-Octen-*3*-yl propionate
233 *beta*-Octenyl propionate
2362 *1*-Octenyl cyanide
2439 *1*-Octin
2400 *n*-Octoic acid
2408 .... *n*-Octyl acetate
2041 "*iso*-Octyl acetate" (see also 1262)
2406 "*secondary*"-Octyl acetate
3066 *3*-Octyl acrolein
1265 *iso*-Octyl acrylate
2401 *n*-Octyl alcohol
2058 "*iso*-Octyl alcohol"
2057 *secondary*-Octyl alcohol
2397 Octyl aldehyde
2398 Octyl aldehyde diethyl acetal
2399 Octyl aldehyde dimethyl acetal
2409 *n*-Octyl-*2*-aminobenzoate
2409 .... *n*-Octyl anthranilate
2410 .... Octyl benzoate
2411 .... Octyl-*n*-butyrate
2412 .... Octyl-*iso*-butyrate
2413 .... *secondary*-Octyl-*iso*-butyrate
2414 .... *alpha*-Octyl-*gamma*-butyrolactone
1102 *gamma*-*n*-Octyl-*gamma*-*n*-butyrolactone
2415 .... Octyl caproate
2416 .... *n*-Octyl caprylate
2348 Octyl carbinol
2417 .... Octyl cinnamate
2418 .... *alpha*-*n*-Octyl cinnamic aldehyde
2346 "Octyl crotonyl acetate"
2419 .... *para*-Octyl cyclohexanone
2420 .... *alpha*-Octyl cyclopentanone
2421 .... Octylene
2421 *alpha*-Octylene
1319 Octyl ethyl ketone
2422 .... *n*-Octyl formate
2059 *secondary*-Octyl formate
2424 *n*-Octylfuran-*alpha*-carboxylate
2423 .... *alpha*-Octyl furfuracrolein
2424 .... *n*-Octyl furoate
2423 *alpha*-*n*-Octyl-*beta*-*2*-furylacrolein
2426 Octyl heptanoate
2425 .... Octyl heptin carbonate
2426 .... Octyl heptoate
2426 Octyl heptylate
1555 Octyl heptyl ether
2415 Octyl hexanoate
2415 Octyl hexoate
2415 Octyl hexylate
2436 *n*-Octyl-*ortho*-hydroxybenzoate
2400 *n*-Octylic acid
2427 .... Octylidene acetone
2428 .... *alpha*-Octylidene cyclopentanone
2395 *iso*-Octyllactone
2429 .... *n*-Octyl malonate
2422 Octyl methanoate
2438 *n*-Octyl-*3*-methylbutyrate
2146 Octyl methyl ketone
2431 Octyl nonanoate
2431 Octyl nonylate
2416 Octyl octanoate
2416 Octyl octoate

2416 Octyl octylate
2425 *n*-Octyl octynoate
2426 "Octyl oenanthate"
2430 .... *n*-Octyl oxyacetaldehyde
2431 .... Octyl pelargonate
2437 *n*-Octyl-*n*-pentanoate
2432 .... Octyl phenol
2432 *para*-Octyl phenol
2433 .... *n*-Octyl phenylacetate
2434 .... *n*-*secondary*-Octyl phenylacetate
3038 *3*-*n*-Octyl-*2*-propen-*1*-ol
2435 .... Octyl propionate
2424 *n*-Octyl pyromucate
2436 .... Octyl salicylate
2433 *n*-Octyl-*alpha*-toluate
2437 .... Octyl-*n*-valerate
2438 .... *n*-Octyl-*iso*-valerate
2982 *alpha*-*n*-Octyl-*delta*-valerolactone
2439 .... Octyne
1494 Oenanthal
1513 Oenanthic acetate
1500 Oenanthic acid
1494 Oenanthic aldehyde
1321 "Oenanthic ether" (see also 1513 and 1545)
1494 "Oenanthol" (so-called)
922 "Oenanthone"
1546 Oenanthylidene acetone
1549 Oenanthylidene methylanthranilate
2440 .... Oleic acid
2440 Oleinic acid
2938 "Onion lachrymator"
2660 Optal
2397 "Orange aldehyde"
2124 "Orangeol"
2124 "Oranger crystals"
2123 "Oranger liquide"
218 "Orchidée"
2796 *beta*-Orcin
2441 .... Orcinol dimethylether
2442 .... Orcinol monomethylether
2419 "Ordilon"
2124 "Orenolia"
2876 Origanol
166 "Orivone"
2288 Orris butter
2288 Orris concrete oil
440 "Oryclon"
2443 .... *10*-Oxahexadecanolide
2444 .... *11*-Oxahexadecanolide
2445 .... *12*-Oxahexadecanolide
2443 "Oxalide"
1256 *3*-Oxanonane
1760 Oxanone
972 "Oxanthin"
1758 *4*-Oxa-tetradecanolide
616 *1,8*-Oxido-*para*-menthane
1226 Oxirane
39 *2'*-Oxo-*2*-ethylfuran
1532 *1*-Oxo-*4*-heptylcyclohexane
1654 *1*-Oxo-*4*-hexylcyclohexane
1655 *1*-Oxo-*2*-*iso*-hexylcyclohexane
1656 *1*-Oxo-*4*-*iso*-hexylcyclohexane
1412 Oxole
1413 *2'*-Oxo-*2*-methylfuran
2446 .... *1*-Oxo-*2*-methyl-*2*-(*para*-*iso*-propylphenyl)-ethane
2343 *alpha*-Oxononane
2373 *1*-Oxo-*4*-nonyl cyclohexane
2419 *1*-Oxo-*4*-octylcyclohexane
1798 *gamma*-Oxopentanoic acid
2470 *1*-Oxo-*2*-phenylethane
2786 *2*-Oxopropanal
2785 *2*-Oxopropanoic acid
3028 *alpha*-Oxo-undecane
2140 *beta*-Oxo-undecane
1798 *4*-Oxovaleric acid
1798 *gamma*-Oxovaleric acid
2944 *alpha*-Oxycymol
1728 Oxydihydrocitronellal
2513 $1^2$-Oxy-*1*-ethylbenzol
1531 *1*-Oxy-*4*-heptyl cyclohexane
1574 *alpha*-Oxy hexadecane
1472 *1*-Oxy-*2*-methoxybenzene
1695 *4*-Oxy-*3*-methoxy phenylacetaldehyde
2077 "Oxymethylacetophenone"
2216 *2*-Oxy-*3*-methyl-*4*(*4'*-*iso*-propylcyclohexyl)-butane-*3*
1760 "Oxyphenylon"
811 *14*-Oxy-tetradecane carbonic acid. lactone

**P**

2485 P.A.D.M.A.
433 "Padoryl"
1747 "Paeonal"
1747 "Paeonol"
1051 "Palatinol M"
1831 Palatone
1573 Palmitaldehyde
2447 .... Palmitic acid
1573 Palmitic aldehyde
1574 Palmityl alcohol
2192 Pandanus oil
2650 Paranol
1688 Paranol ethylether
2339 "Parmantheme"
2448 .... Parmavert
261 Parsley apiole
433 "Patchone"
614 P.C.M.X.
2513 P.E.A.
3024 "Peach aldehyde"
828 "Peachtone"
119 "Pear ether"
119 "Pear oil"
2132 "Pekleol"
1032 "Pelargol"
2350 *gamma*-Pelargolactone
2343 Pelargonaldehyde
2344 Pelargonaldehyde diethyl acetal
2345 Pelargonaldehyde dimethyl acetal
2347 Pelargonic acid
2355 Pelargonic acid, piperidide
2348 Pelargonic alcohol
2343 Pelargonic aldehyde
1312 Pelargonic ether
2355 Pelargonic piperidide
2363 Pelargonyl acetate
2355 Pelargonyl piperidine
2353 Pelargonyl vanillylamide

2541 P.E.M.E.C.
2628 Pennyroyal oil, Moroccan
1465 Penta-acetyl-*alpha*-*dextro*-glucose
1465 *beta*-Penta-acetyl-*dextro*-glucose
2449 .... Pentadecanal
811 *omega*-Pentadecalactone
2450 .... Pentadecanol
811 Pentadecanolide (see also 3048)
2451 .... Pentadecyl acetate
2450 *n*-Pentadecyl alcohol
2449 Pentadecyl aldehyde
194 "Pentalarm" (see also 1673)
3053 *iso*-Pentaldehyde
811 "Pentalide"
1791 *4,7,7,10,10*-Pentamethyl-(*4,4,0*)-bicyclodecan-*3*-one
2275 *1,1,3,3,5*-Pentamethyl-*4,6*-dinitroindan
2626 Pentamethylenimine
3052 *n*-Pentanal
3053 *iso*-Pentanal
1177 Pentane-*3*-carboxaldehyde
1596 Pentane-*1*-carboxylic acid
2265 Pentane-*2*-carboxylic acid
1180 Pentane-*3*-carboxylic acid
45 *2,3*-Pentanedione
29 *2,4*-Pentanedione
194 *1*-Pentane thiol
3056 Pentanoic acid
3057 *iso*-Pentanoic acid (see also 1941)
125 *1*-Pentanol
127 *2*-Pentanol
3059 Pentanolide-*1 : 4*
2226 *2*-Pentanone
2653 *3*-Pentanone
120 *2*-Pentanyl acetate
205 Pentaphen
2453 *4*-Pentene nitrile
2452 .... *4*-Pentenoic acid
2453 .... Pentenoic acid, nitrile
2454 .... *beta*-Pentenol
2454 *1*-Penten-*3*-ol
1924 "*iso*-Pentenol"
2951 Pentenoyl piperidide
2455 .... *beta*-Pentenyl acetate
2455 *1*-Penten-*3*-yl acetate
2393 Pentenyl acrolein
2093 *2*-Pentenyl cyclopentanone-*3*-acetic acid, methylester
2094 *2*-*iso*-Pentenyl cyclopentanone-*3*-acetic acid, methylester
2093 *2*-(*cis*-Penten-*2'*-yl)-*3*-oxo-cyclopentane-acetic acid, methylester
1787 *cis*-*5*-(*2*-Pentenyl pentanolide-*5 : 1*)
2456 .... Pentione
170 *1*-Pentoxy-*2*-methoxy-*4*-allylbenzene
171 *1*-Pentoxy-*2*-methoxy-*4*-propenylbenzene
1762 *beta*-*iso*-Pentoxypropionic aldehyde
1764 *beta*-*iso*-Pentoxypropionaldehyde diethylacetal
119 *iso*-Pentylacetate
124 *2*-Pentyl acrolein
2407 *n*-Pentyl acrylic acid
125 Pentyl alcohol
126 *iso*-Pentyl alcohol
131 *iso*-Pentyl-*ortho*-aminobenzoate
132 *iso*-Pentyl benzoate
137 *iso*-Pentyl-*n*-butanoate
136 Pentyl butyrate
137 *iso*-Pentyl-*n*-butyrate
138 *iso*-Pentyl-*iso*-butyrate
139 *2*-Pentyl butyrate
147 *iso*-Pentyl cinnamate
158 *alpha*-Pentyl cinnamyl acetate
148 *alpha*-Pentyl cinnamyl alcohol
159 *alpha*-Pentyl cinnamyl formate
161 *alpha*-Pentyl cinnamyl-*iso*-valerate
219 *iso*-Pentyl decane dioate
141 *iso*-Pentyl decanoate
141 *iso*-Pentyl decylate
191 *iso*-Pentyl dodecanoate
169 *iso*-Pentyl ether
172 *n*-Pentyl formate
173 *iso*-Pentyl formate
174 *iso*-Pentyl-*2*-furanbutyrate
179 *iso*-Pentylfuran-*alpha*-carboxylate
175 *iso*-Pentyl-*2*-furanpropionate
178 Pentyl-*2*-furoate
183 Pentyl heptoate
184 *iso*-Pentyl heptoate
142 Pentyl hexanoate
143 *iso*-Pentyl-*n*-hexanoate
218 *iso*-Pentyl-*ortho*-hydroxybenzoate
190 *iso*-Pentyl-*beta*-hydroxypropionate
2457 .... *2*-*n*-Pentylidene cyclohexanone-*1*
3059 Pentyllactone
129 *iso*-Pentyl-*cis*-*2*-methylbutyrate
225 *iso*-Pentyl-*trans*-*alpha*-methylcrotonate
954 *2*-Pentyl-*3*-methyl-*2*-cyclopenten-*1*-one
200 *iso*-Pentyl nonanoate
201 *iso*-Pentyl nonynoate
144 Pentyl octoate
145 *iso*-Pentyl octylate
2839 *2*-(Pentylol-*2'*)-cyclohexen-*2*-carboxylic acid-*1*
2841 *2*-(Pentylon-*2'*)-cyclohexen-*6*-carboxylic acid-*1*
228 *n*-Pentyl-*n*-pentanoate
208 *n*-Pentyl phenylacetate
208 *iso*-Pentyl phenylacetate
149 *alpha*-Pentyl-*beta*-phenylacrolein
147 *iso*-Pentyl-*beta*-phenylacrylate
147 *iso*-Pentyl-*3*-phenylpropenoate
186 *alpha*-*n*-Pentyl phenylpropyl alcohol
213 *iso*-Pentyl propionate
217 *iso*-Pentyl pyruvate
218 *iso*-Pentyl salicylate
197 *iso*-Pentyl tetradecanoate
226 *iso*-Pentyl undecanoate
227 *iso*-Pentyl undecenoate
229 *iso*-Pentyl-*iso*-valerate
231 *n*-Pentyl vinyl carbinol
232 *n*-Pentyl vinyl carbinyl acetate
233 *n*-Pentyl vinyl carbinyl propionate
1747 "Peonol"
1428 "Peony aldehyde"

1747 "Peony ketone"
2548 P.E.P.A.
12 Pepital
1840 "Peppermint camphor"
1571 Perchloroethane
936 Perilla alcohol
937 Perilla aldehyde
938 *laevo*-Perilla-aldehyde-*alpha*-anti-aldoxim
938 "Perillartine"
935 Perillyl acetate
936 Perillyl alcohol
265 *1*,*4*-Peroxido-*para*-menthene-*2*
3024 "Persicol"
2316 "Peruviol"
938 "Peryllartine"
2661 Petrohol
2696 P.G.
40 "Phantolide"
2458 .... Phellandral
2459 .... *alpha*-Phellandrene
2460 .... *beta*-Phellandrene
2513 Phenarose
1335 Phenethole
1125 *para*-Phenethole carbamide
2461 .... Phenethoxy acetaldehyde
2512 *beta*-Phenethyl acetate
2513 *beta*-Phenethyl alcohol
2514 *beta*-Phenethyl-*ortho*-aminobenzoate
2515 *beta*-Phenethyl benzoate
2516 *beta*-Phenethyl butanoate
2523 *beta*-Phenethyl-*trans*-*2*-butenoate
2517 *beta*-Phenethyl-*iso*-butyrate
2589 Phenethyl carbinol
2545 *beta*-Phenethyl chloracetate
2522 *beta*-Phenethyl cinnamate
2525 *beta*-Phenethyl diethylacetate
2552 *beta*-Phenethyl-*3*,*3*-dimethylacrylate
1704 *2*-*alpha*-Phenethyl-*1*,*3*-dioxolane
2585 *2*-*beta*-Phenethyl-*1*,*3*-dioxolane
2530 *beta*-Phenethyl furoate
2531 *beta*-Phenethyl heptanoate
2518 *beta*-Phenethyl hexoate
2551 *beta*-Phenethyl-*ortho*-hydroxybenzoate
2533 *beta*-Phenethyl-*2*-hydroxypropanoate
2534 *beta*-Phenethyl laevulate
2554 *beta*-Phenethyl-*2*-mercapto ethanoate
2529 *beta*-Phenethyl methanoate
2537 *beta*-Phenethyl-*alpha*-methylbutanoate
2535 *beta*-Phenethyl methylpropenoate
2553 "*beta*-Phenethyl mustard oil"
2547 *beta*-Phenethyl nonanoate
2519 *beta*-Phenethyl octoate
2513 Phenethylol
2557 *beta*-Phenethyl-*n*-pentanoate
2558 *beta*-Phenethyl-*iso*-pentanoate
2549 *beta*-Phenethyl propanoate
2740 Phenethyl propylether
2553 *beta*-Phenethyl thiocarbimide
2555 *beta*-Phenethyl tiglate
2548 *beta*-Phenethyl-*alpha*-toluate
2582 *2*-Phenethyl-*4*,*4*,*6*-trimethyl-*1*,*3*-dioxan
2556 *beta*-Phenethyl undecenoate
1125 *para*-Phenethyl urea
2466 "Phenirat"
2303 Phenol naphthylether
2462 .... Phenoxy acetaldehyde
2463 Phenoxy acetaldehyde-*tertiary*-butyl acetal
2463 .... Phenoxy acetaldehyde diethyl acetal
2463 Phenoxy acetaldehyde dimethyl acetal
2463 Phenoxy acetaldehyde ethyl butyl acetal
2464 .... Phenoxyacetic acid
1330 Phenoxyacetic acid, ethylester
2464 Phenoxyethanoic acid
1223 *2*-Phenoxyethanol
2465 .... Phenoxyethyl acetate
1223 *beta*-Phenoxyethyl alcohol
2466 Phenoxyethyl-*n*-butyrate
2466 .... Phenoxyethyl-*iso*-butyrate
2467 .... Phenoxyethyl propionate
2468 .... Phenoxyethyl-*iso*-valerate
1766 *beta*-Phenoxypropionic aldehyde diethyl acetal
2469 .... Phenoxy propyl butyrate
2470 .... Phenylacetaldehyde
2471 .... Phenylacetaldehyde-*2*,*3*-butyleneglycol acetal
2472 .... Phenylacetaldehyde citronellyl methyl acetal
2473 .... Phenylacetaldehyde citronellyl phenylethyl acetal
327 Phenylacetaldehyde cyclic acetal of glycerin methylether
2474 .... Phenylacetaldehyde diallyl acetal
2475 .... Phenylacetaldehyde diamyl acetal
2476 .... Phenylacetaldehyde di-benzyl acetal
2477 .... Phenylacetaldehyde di-butyl acetal
2477 Phenylacetaldehyde di-*iso*-butyl-acetal
2478 .... Phenylacetaldehyde di-citronellyl acetal
2479 .... Phenylacetaldehyde diethyl acetal
2480 .... Phenylacetaldehyde di-geranyl acetal
2481 .... Phenylacetaldehyde-*1*,*2*-dihydroxybutane acetal
2482 .... Phenylacetaldehyde-*1*,*3*-dihydroxybutane acetal
2483 .... Phenylacetaldehyde-*2*,*4*-dihydroxy-*4*-methylpentane acetal
2484 .... Phenylacetaldehyde-*1*,*2*-dihydroxypropane acetal
2485 .... Phenylacetaldehyde dimethyl acetal
2486 Phenylacetaldehyde di-propyl acetal
2486 .... Phenylacetaldehyde di-*iso*-propyl acetal
2487 Phenylacetaldehyde ethylene acetal
2487 .... Phenylacetaldehyde ethyleneglycol acetal
327 Phenylacetaldehyde glycerin-methylether, cyclic acetal
2488 .... Phenylacetaldehyde glyceryl acetal
2489 .... Phenylacetaldehyde monobenzyl acetal

2490 .... Phenylacetaldehyde phenylethyleneglycol acetal
2470 Phenylacetaldehyde-"polymer"
2484 Phenylacetaldehyde propyleneglycol acetal
2491 .... Phenyl acetate
2492 .... Phenylacetic acid
1920 Phenylacetone
302 Phenylacetonitrile
2493 *para*-Phenylacetophenone
2493 .... Phenyl acetyl benzol
2494 .... Phenyl acetylene
619 *gamma*-Phenylacrolein
617 *trans-beta*-Phenylacrylic acid
2495 .... *alpha*-Phenyl allyl acetate
626 *trans-gamma*-Phenyl allyl acetate
2496 .... *alpha*-Phenyl allyl alcohol
618 *gamma*-Phenyl allyl alcohol
633 Phenyl allyl cinnamate
2497 .... Phenyl allyl ether
644 *gamma*-Phenyl allyl propionate
240 Phenylamine
2499 Phenyl-*2*-aminobenzoate
2498 .... Phenyl amylalcohol
2006 *ortho*-Phenylanisole
2499 .... Phenyl anthranilate
2500 .... Phenyl benzoate
1077 Phenyl benzol
2501 .... *2*-Phenyl benzothiazole
2501 *2*-Phenyl-(*1,3*-benzthiazole)
334 Phenyl benzyl carbinol
335 Phenyl benzyl carbinyl acetate
2490 *4*-Phenyl-*2*-benzyl-*1,3*-dioxolan
336 Phenyl benzyl ether
2609 Phenyl-*1,3*-butadiene methylketone
2506 *gamma*-Phenyl-*n*-butanal
2506 *4*-Phenylbutanal
283 *4*-Phenylbutan-*2,4*-dione
2505 *4*-Phenylbutanoic acid
2502 .... *3*-Phenyl-*1*-butanol
2503 *4*-Phenylbutanol-*1*
2538 *dl-4*-Phenyl-*2*-butanol
2539 *4*-Phenyl-*2*-butanol acetate
2540 *4*-Phenyl-*2*-butanol-*iso*-valerate
288 *4*-Phenylbutan-*2*-one
1691 *4*-Phenyl-*3*-buten-*2*-ol
318 *4*-Phenyl-*3*-buten-*2*-one
2503 .... Phenyl butyl alcohol (see also 2502)
2503 *gamma*-Phenyl-*n*-butylalcohol
989 Phenyl-*tertiary*-butylalcohol
511 Phenyl-*n*-butylcarbinol
512 Phenyl-*iso*-butylcarbinol
513 Phenyl-*iso*-butylcarbinyl acetate
514 Phenyl-*iso*-butylether
3060 Phenyl butyl ketone
3061 Phenyl-*iso*-butyl ketone
2506 *gamma*-Phenyl butyraldehyde
2504 .... Phenyl-*iso*-butyrate
2505 .... Phenylbutyric acid
2174 *gamma*-Phenylbutyric acid, methylester
2506 .... Phenylbutyric aldehyde
2597 Phenylbutyric nitrile
2507 .... Phenyl butyrolactone
2507 *alpha*-Phenyl-*gamma*-butyrolactone
2507 *gamma*-Phenyl-*gamma*-butyrolactone
2597 Phenyl butyronitrile
2510 Phenylcarbimide
290 Phenylcarbinol
2510 Phenylcarbonimide
1223 Phenylcellosolve
2465 Phenylcellosolve acetate
2466 Phenylcellosolve-*iso*-butyrate
2467 Phenylcellosolve propionate
2468 Phenylcellosolve-*iso*-valerate
2508 .... Phenyl cinnamate
2508 *alpha*-Phenylcinnamic acid
2509 .... Phenylcinnamic aldehyde
319 Phenylcinnamyl ketone
722 "Phenyl cresyl ether"
720 Phenyl-*meta*-cresyl oxide
721 Phenyl-*ortho*-cresyl oxide
722 Phenyl-*para*-cresyl oxide
2510 .... Phenyl-*iso*-cyanate
279 Phenyl cyanide
893 Phenyl dichloro nitroethylene
1040 Phenyl dimethyl carbinol
1041 Phenyl dimethyl carbinyl acetate
1042 Phenyl dimethyl carbinyl-*iso*-butyrate
1409 *4*-Phenyl-*1,3*-dioxacyclopentane
272 *2*-Phenyl-*1,3*-dioxolan
1409 *4*-Phenyl-*meta*-dioxolan
1157 Phenylethane
2563 *1*-Phenylethanediol-*1 : 2*
2524 Phenyl-*1,2*-ethanediol diphenylacetate
2574 Phenyl-*1,2*-ethanediol monophenylacetate
2513 *beta*-Phenylethanol
2175 *1*-Phenylethan-*1*-ol
1081 Phenylether
1336 Phenylethoxyacetic acid, ethylester
2511 .... Phenylethyl acetal
2512 .... Phenylethyl acetate
2176 *alpha*-Phenyl ethyl acetate
2176 *secondary*-Phenyl ethyl acetate
2513 .... Phenylethyl alcohol
2175 *alpha*-Phenyl ethyl alcohol
210 Phenylethyl-*iso*-amylether
2514 .... Phenylethyl anthranilate
2515 .... Phenylethyl benzoate
337 Phenylethyl benzylether
369 *alpha*-Phenylethyl bromide
898 *1*-Phenyl-*2*-ethyl-*1*-butanone
2516 .... Phenylethyl butyrate
2517 .... Phenylethyl-*iso*-butyrate
2518 .... Phenylethyl caproate
2519 .... Phenylethyl caprylate
2520 .... Phenylethyl carbinol
2521 .... Phenylethyl carbinyl acetate
2522 .... Phenylethyl cinnamate (see also 2508)
2523 .... Phenylethyl crotonate
2586 Phenylethyl cyanide
1043 Phenylethyl dimethylcarbinol
1044 Phenylethyl dimethyl carbinyl acetate
1045 Phenylethyl dimethyl carbinyl-*n*-butyrate

1046 Phenylethyl dimethyl carbinyl-*iso*-butyrate
1047 Phenylethyl dimethyl carbinyl formate
1048 Phenylethyl dimethyl carbinyl propionate
1049 Phenylethyl dimethyl carbinyl-*iso*-valerate
1703 *2-alpha*-Phenyl ethyl-*1,3*-dioxane
2865 Phenylethylene
2176 "Phenylethylene acetate"
2570 Phenylethyleneglycol benzoate
2566 Phenylethyleneglycol diacetate, *primary*
2567 Phenylethyleneglycol diformate
2524 .... Phenylethyleneglycol diphenylacetate
2571 Phenylethyleneglycol-*primary*-mono-*n*-butanoate
2565 Phenylethyleneglycol-*primary*-monocinnamate
2573 Phenylethyleneglycol-*primary*-mono-*iso*-valerate
2572 Phenylethyleneglycol propanoate
2574 Phenylethyleneglycol-*alpha*-toluate
2866 Phenylethylene oxide
1335 Phenyl ethyl ether
2525 .... Phenylethyl-*2*-ethylbutyrate
2526 .... Phenylethyl ethyl carbinol
2527 .... Phenylethyl ethyl carbinyl acetate
2528 .... Phenylethyl ethyl carbonate
1338 Phenylethyl ethyl ether
2560 Phenylethyl-*iso*-eugenol
2529 .... Phenylethyl formate
2530 .... Phenylethyl-*2*-furoate
2531 .... Phenylethyl heptoate
2531 Phenylethyl heptylate
1560 Phenylethyl heptyl ether
2518 Phenylethyl hexanoate
306 *1*-Phenyl-*2*-ethyl-*3*-hexanone
1678 Phenylethyl hexyl carbinol
2532 .... Phenylethylidene acetone
2656 Phenylethyl ketone
2534 Phenylethyl-*gamma*-ketovalerate
2533 .... Phenylethyl lactate
2534 .... Phenylethyl levulinate
2535 .... Phenylethyl methacrylate
2536 .... Phenylethyl methoxyacetate
2555 Phenylethyl-*alpha*-methylbutenoate
2537 .... Phenylethyl-*2*-methylbutyrate
2558 Phenylethyl-*3*-methylbutyrate
2538 .... Phenylethyl methylcarbinol
2539 .... Phenylethyl methyl carbinyl acetate
2540 .... Phenylethyl methyl carbinyl-*iso*-valerate
2552 Phenylethyl-*3*-methylcrotonate
2192 Phenylethyl methyl ether
2541 .... Phenylethyl methyl ethyl carbinol
2542 .... Phenylethyl methyl ethyl carbinyl acetate
2543 .... Phenylethyl methyl ethyl carbinyl propionate
2544 .... Phenylethyl methyl ethyl carbinyl-*iso*-valerate
288 *beta*-Phenylethyl methyl ketone
2545 .... Phenylethyl monochloroacetate
2519 Phenylethyl octanoate
2546 .... Phenylethyl oxalate
2461 Phenylethyl oxyacetaldehyde
2547 .... Phenylethyl pelargonate
2548 .... Phenylethyl phenylacetate
2522 *beta*-Phenylethyl-*3*-phenylpropenoate
2549 .... Phenylethyl propionate
2550 .... Phenylethyl-*iso*-propoxy acetate
2198 Phenylethyl-*iso*-propyl carbinol
2740 Phenylethyl propyl ether
969 *alpha*-Phenylethyl pyridine
2551 .... Phenylethyl salicylate
2552 .... Phenylethyl senecioate
2924 Phenylethyl tetrahydro-*2*-pyranyl-ether
2553 .... Phenylethyl-*iso*-thiocyanate (see also 2510)
2554 .... Phenylethyl thioglycolate
2555 .... Phenylethyl tiglate
1701 *2-alpha*-Phenylethyl-*4,4,6*-trimethyl-*1,3*-dioxane
2556 .... Phenylethyl undecylenate
2557 .... Phenylethyl valerate
2558 .... Phenylethyl-*iso*-valerate
2559 .... Phenylethyl vinylether
2560 .... Phenyl-*iso*-eugenol
2561 .... Phenyl formate
276 Phenylformic acid
2562 .... *beta*-Phenylglycidic acid
2563 .... Phenyl glycol
11 Phenyl glycol acetal
1409 "Phenyl glycol acetal" (so-called)
2564 .... Phenylglycol anthranilate
2565 .... Phenylglycol cinnamate
2566 .... Phenylglycol diacetate
2567 .... Phenylglycol formate
2464 *O*-Phenylglycolic acid
1409 Phenylglycol methylene acetal
1409 Phenylglycol methylene ether
2568 ... *primary*-Phenylglycol monoacetate
2569 .... *secondary*-Phenylglycol monoacetate
2570 .... Phenylglycol monobenzoate
2571 .... Phenylglycol monobutyrate
2572 .... Phenylglycol monopropionate
2573 .... Phenylglycol mono-*iso*-valerate
2574 .... Phenylglycol phenylacetate
2572 *primary*-Phenylglycol propanoate
2575 *6*-Phenylheptanol-*2*
2575 .... Phenyl heptyl alcohol
1559 Phenyl heptyl ether
2609 *1*-Phenylhexa-*1,3*-dien-*5*-one
2609 *6*-Phenyl-*3,5*-hexadien-*2*-one
55 *1*-Phenyl-*2,4*-hexadiyne
554 *1*-Phenylhexane-*1,3*-dione
2576 *1*-Phenylhexanol-*5*
2576 *primary-1*-Phenylhexanol-*6*
1706 *5*-Phenylhexan-*2*-one
2576 .... Phenyl hexyl alcohol
2200 Phenyl-*active*-hexylalcohol
2607 Phenyl-*ortho*-hydroxybenzoate
1272 *2*-Phenyl-*2*-hydroxy ethylpropionate
2195 *2*-Phenyl-*2*-hydroxy undecane
2464 Phenylium

2937 Phenylmercaptan
2952 Phenyl methane
290 Phenyl methanol
2560 Phenyl-*2*-methoxy-*4*-propenyl phenylether
2670 *1*-Phenyl-*3*-methyl-*2*-butanol
2671 *1*-Phenyl-*3*-methyl-*2*-butanol acetate
2175 Phenyl methyl carbinol
2176 Phenyl methyl carbinyl acetate
2180 Phenyl methyl carbinyl-*iso*-butyrate
2184 Phenyl methyl carbinyl formate
2181 Phenyl methyl carbinyl hexoate
2186 Phenyl methyl carbinyl propionate
2187 Phenyl methyl carbinyl salicylate
2188 Phenyl methyl carbinyl-*iso*-valerate
246 Phenyl methyl ether
2021 Phenyl methyl ethyl carbinol
2022 Phenyl methyl ethyl carbinyl acetate
321 *1*-Phenyl-*5*-methyl-*1*,*4*-heptadien-*3*-one
24 Phenyl methyl ketone
2541 *1*-Phenyl-*3*-methyl-*3*-pentanol
2542 *1*-Phenyl-*3*-methyl-*3*-pentanol acetate
2543 *1*-Phenyl-*3*-methyl-*3*-pentanol propionate
2544 *1*-Phenyl-*3*-methyl-*3*-pentanol-*iso*-valerate
2006 *ortho*-Phenyl methyl phenyl ether
2577 .... Phenyl naphthyl ketone
2303 "Phenyl naphthyl oxide"
1678 9-Phenylnonanol-*7*
2580 "Phenylone"
2559 *5*-Phenyl-*3*-oxopent-*1*-ene
320 *3*-Phenyl-*2*,*4*-pentadienal
2669 *1*-Phenyl-*2*-pentanol
2498 *5*-Phenylpentanol-*1*
2526 *5*-Phenylpentan-*3*-ol
2669 *5*-Phenylpentan-*4*-ol
3060 *1*-Phenyl-*1*-pentanone
1916 *2*-Phenylpentan-*4*-one
328 *5*-Phenyl-*2*-pentanone
2527 *5*-Phenylpentan-*3*-yl acetate
2532 *5*-Phenyl-*3*-penten-*2*-one
1696 *2*-Phenylpropanal
2580 *3*-Phenylpropanal
2665 *1*-Phenylpropane
2520 *1*-Phenyl-*1*-propanol
1917 *1*-Phenylpropan-*2*-ol
1707 *2*-Phenylpropan-*1*-ol
2589 *3*-Phenyl-*1*-propanol
2656 *1*-Phenyl-*1*-propanone
1920 *3*-Phenyl-*2*-propanone
619 *3*-Phenylpropenal
617 *trans*-*3*-Phenylpropenoic acid
2496 *1*-Phenyl-*2*-propen-*1*-ol
618 *3*-Phenyl-*2*-propen-*1*-ol
2495 *1*-Phenyl-*2*-propen-*1*-yl acetate
629 Phenyl propenyl-*n*-butyrate
644 *3*-Phenyl-*2*-propenyl propanoate
1696 *alpha*-Phenyl propionaldehyde
2580 *beta*-Phenyl propionaldehyde
1700 *2*-Phenylpropionaldehyde dimethyl acetal
2578 .... *alpha*-Phenyl propionic acid
2578 *beta*-Phenyl propionic acid (see also 2579)
2579 *gamma*-Phenyl propionic acid
2578 *2*-Phenyl propionic acid
2579 .... *3*-Phenyl propionic acid
2586 Phenylpropionic acid, nitrile
2580 .... *3*-Phenylpropionic aldehyde
2581 .... *3*-Phenylpropionic aldehyde diethyl acetal
2582 .... *3*-Phenylpropionic aldehyde-*2*,*4*-dihydroxy-*4*-methylpentane acetal
2583 .... *3*-Phenylpropionic aldehyde dimethyl acetal
2584 .... *3*-Phenylpropionic aldehyde diphenylethyl acetal
2585 .... *3*-Phenylpropionic aldehyde ethyleneglycol acetal
2586 .... Phenyl propionitrile
2587 .... Phenyl propoxyacetic acid
1341 Phenylpropoxyacetic acid, ethylester
1705 *2*-Phenyl propyl acetate
2588 .... *3*-Phenyl propyl acetate
1705 *alpha*-Phenyl propyl acetate
1041 Phenyl-*iso*-propyl acetate
2588 *beta*-Phenyl propyl acetate
2521 *secondary*-Phenyl propyl acetate
2589 .... *3*-Phenyl propyl alcohol
1707 *alpha*-Phenyl propyl alcohol
2589 *beta*-Phenyl propyl alcohol (see also 1707)
2589 *gamma*-Phenyl propyl alcohol
1040 Phenyl-*iso*-propylalcohol
2520 *secondary*-Phenyl propyl alcohol
2590 .... *3*-Phenyl propyl benzoate
1165 *alpha*-Phenyl propyl butyrate
2591 .... *3*-Phenyl propyl butyrate
2592 .... *3*-Phenyl propyl-*iso*-butyrate
2591 "*beta*"-Phenyl propyl butyrate
2592 "*beta*"-Phenyl propyl-*iso*-butyrate
1708 *2*-Phenylpropyl-*n*-butyrate
1709 *2*-Phenylpropyl-*iso*-butyrate
2593 .... *3*-Phenyl propyl caprinate
2594 .... *3*-Phenyl propyl caproate
2595 .... *3*-Phenyl propyl caprylate
990 Phenyl-*iso*-propylcarbinol
2596 "*beta*"-Phenylpropyl cinnamate
2596 .... *3*-Phenyl propyl cinnamate
2597 .... *3*-Phenyl propyl cyanide
2593 "*beta*"-Phenylpropyl decanoate
2598 "*beta*"-Phenylpropyl formate
2598 .... *3*-Phenyl propyl formate
2594 "*beta*"-Phenylpropyl hexoate
2595 Phenylpropyl hexylate
553 Phenyl-*n*-propyl ketone
2598 *3*-Phenyl-*1*-propyl methanoate
2605 *3*-Phenylpropyl-*beta*-methylbutyrate
2203 *beta*-Phenylpropyl methylether
1706 *alpha*-Phenylpropyl methyl ketone
2595 Phenylpropyl octylate
2604 *2*-Phenylpropyl-*n*-pentanoate
2599 "*beta*"-Phenylpropyl phenylacetate
2599 .... *3*-Phenyl propyl phenylacetate
2600 *3*-Phenylpropyl propanoate
1706 *alpha*-Phenylpropyl propanone

2600 "*beta*"-Phenylpropyl propionate
2600 .... *3*-Phenyl propyl propionate
2601 .... *alpha*-(*3*-Phenyl propyl)-pyridine
2601 *gamma*-Phenyl propyl pyridine
2601 *ortho*-Phenyl propyl pyridine
2602 *alpha*-(*3*-Phenyl propyl)-tetrahydrofuran
2602 .... *2*-(*3*-Phenyl propyl)-tetrahydrofuran
2603 .... *3*-Phenyl propyl undecylenate
2604 .... *3*-Phenyl propyl valerate (see also 2605)
2605 .... *3*-Phenyl propyl-*iso*-valerate
2606 .... *alpha*-Phenyl pyridine
2606 *gamma*-Phenyl pyridine
2606 *2*-Phenyl pyridine
2606 *4*-Phenyl pyridine
2607 .... Phenyl salicylate
319 Phenyl styryl ketone
721 Phenyl-*ortho*-tolylether
722 Phenyl-*para*-tolylether
1913 Phenyl-*ortho*-tolyl ketone
2195 *2*-Phenyl-*2*-undecanol
2608 .... Phenyl vinyl acetate
2608 *beta*-Phenyl vinylacetate
2496 Phenyl vinyl carbinol
2495 Phenyl vinyl carbinyl acetate
2609 .... Phenyl vinylethylene methylketone
510 Phenysol
1728 "Phixia"
1741 Phloracetophenone dimethylether
981 *2,4*-Phloracetophenone dimethylether
981 *2,6*-Phloracetophenone dimethylether
1328 Phlorol
158 Phloxin acetate (Floxin acetate)
149 Phloxine (Floxine)
159 Phloxine formate
161 Phloxine-*iso*-valerate
440 Phloxyl
2610 .... *iso*-Phorol (see also 967)
2611 .... *iso*-Phorone
2612 .... Phosphoric acid
2612 *ortho*-Phosphoric acid
3097 Phthalan
913 Phthalol
1604 Phyllol (see also 1369)
2613 .... Phytol
2614 .... *iso*-Phytol
2615 .... Phytyl acetate
2775 Piazine
777 Pimelin ketone
2616 .... Pinacol
2617 .... Pinacol dimethylether
2618 "Pinacolin"
2618 .... Pinacolone
2618 Pinacone
2621 *3*-Pinanol
2622 *3*-Pinanone
143 "Pineapple aldehyde"
293 "Pineapple aldehyde C-19"
2619 .... *alpha*-Pinene
2620 .... *beta*-Pinene
2621 .... *dextro*-Pinocampheol
2622 .... Pinocamphone
2623 .... Pinocarveol
2624 .... Pinocarvone
2625 .... Pinol hydrate
604 *alpha-cis-gamma-cis*-Piperic acid
605 *alpha-trans-gamma-cis*-Piperic acid
2626 .... Piperidine
2951 Piperidine tiglate
2627 .... Piperine
2628 .... Piperitenone
2629 .... *iso*-Piperitenone
2630 .... Piperitone
1484 Piperonal
1485 Piperonal diethyl acetal
1486 Piperonal dimethyl acetal
2632 Piperonilic acid
1487 Piperonyl acetate
1488 Piperonyl acetone
1491 Piperonyl acrolein
1489 Piperonyl alcohol
1484 Piperonyl aldehyde
1490 Piperonyl-*iso*-butyrate
2631 .... Piperonyl ethylcarbonate
2632 .... Piperonylic acid
1491 Piperonylidene acetaldehyde
1488 Piperonylidene acetone
2633 .... Piperonylidene diacetate
1342 "Piperonylidene ethylacetate"
2627 *1*-Piperoyl piperidine
2634 .... Polylimonene
86 "Polyone"
2635 Polyoxyethylene(20)sorbitan monolaurate
2635 Polyoxyethylene(20)sorbitan mono-oleate
2635 Polyoxyethylene(20)sorbitan monostearate
2635 Polyoxyethylene(20)sorbitan tristearate
2635 .... Polysorbate
2635 Polysorbate 20
2635 Polysorbate 60
2635 Polysorbate 65
2635 Polysorbate 80
2636 .... Potassium acetate
2637 Potassium acid carbonate
2638 Potassium acid tartrate
2637 .... Potassium bicarbonate
2638 .... Potassium bitartrate
2853 Potassium cyclamate
2639 Potassium-*2,4*-hexadienoate
2638 Potassium hydrogen tartrate
2639 .... Potassium sorbate
1965 "Pralina"
2640 .... Prenol
2641 .... Prenyl acetate
1879 "Primulacamphor"
2155 Primulaverin
436 "Product C-64"
790 "Product C-66"
2710 Progallin
2642 .... Prolin dihydroxyacetone
2652 Propanal
1830 Propanedioic acid
2696 *1,2*-Propanediol
2723 *n*-Propane thiol
1467 *1,2,3*-Propane triol
2654 Propanoic acid

2661 *iso*-Propanol
2660 *1*-Propanol
2661 *2*-Propanol
18 Propanone
287 *2*-Propanone carboxylic acid, benzylester
2643 .... Propargyl alcohol
52 *2*-Propenal
2938 *1*-Propene sulfenic acid
87 *2*-Propene-*1*-thiol
51 *1*-Propene-*1,2,3*-tricarboxylic acid
53 Propenoic acid
63 *1*-Propenyl-*3*-acetate
63 *2*-Propenyl acetate
2858 *2*-Propenyl acrylic acid
84 *2*-Propenyl amylacetylene carboxylate
236 *para*-Propenyl anisole
2644 .... *para-iso*-Propenyl anisole
64 *2*-Propenyl anthranilate
65 *2*-Propenyl benzoate
66 Propenyl benzylether
67 Propenyl butyrate
1859 *iso*-Propenyl carbinyl-*n*-butyrate
1860 *iso*-Propenyl carbinyl caproate
1866 *para*-Propenyl catechol dimethylether
2649 *para*-Propenyl catechol ethyl methyl ether
2814 *4*-Propenyl catechol methylene ether
2018 *4*-Propenyl catechol methyl ethyl ether
72 Propenyl cinnamate
2645 .... Propenyl-*meta*-cresol methylether
1370 Propenyl-*ortho*-cresol methylether
937 *4-iso*-Propenyl cyclohexen-*1*-aldehyde
2208 *ortho*-Propenyl-*para*-cymene
3018 *3*-(*2*-Propen-*1*-yl)-decalol-*1*
3019 *3*-(*2*-Propen-*1*-yl)-decalone-*1*
69 *2*-Propenyl decanoate
262 *1*-(*1*$^2$-Propen-*1*-yl)-*2,5*-dimethoxy-*3,4*-methylene dioxybenzene
63 *2*-Propenyl ethanoate
1688 *1*-Propenyl-*4*-ethoxybenzene
2646 *5*-Propenyl-*2*-ethoxyphenol
79 *2*-Propenyl-*2*-ethylbutyrate
80 *2*-Propenyl ethylcaproate
81 Propenyl formate
2646 .... Propenyl guaethol
1370 *4*-Propenyl guaiacol
2645 *6*-Propenyl guaiacol
1376 *4*-Propenyl guaiacyl phenylacetate
100 *2*-Propenyl hendecenoate
85 Propenyl heptoate
96 *2*-Propenyl-*ortho*-hydroxybenzoate
81 *2*-Propenyl methanoate
2644 *4-iso*-Propenyl-*1*-methoxybenzene
2645 *para*-Propenyl-*meta*-methoxyphenol
1374 *4*-Propenyl-*2*-methoxyphenyl formate
2647 .... *2-iso*-Propenyl-*5*-methylene-*6*-hepten-*1*-ol
2648 .... *2-iso*-Propenyl-*5*-methylene-*6*-hepten-*1*-yl acetate
2649 .... Propenyl methyl guaethol
1794 *2-iso*-Propenyl-*5*-methylhexen-*4*-ol-*1*
88 *2*-Propenyl nonanoate
89 *2*-Propenyl-*2*-nonylenate
71 *2*-Propenyl octanoate
1688 *para*-Propenyl phenethole
2650 .... Propenyl phenol
92 *2*-Propenyl phenylacetate
236 *para*-Propenyl phenyl methylether
2651 .... *2*-Propenyl-*3*-propene thiolsulfinate
93 *2*-Propenyl propionate
96 *2*-Propenyl salicylate
97 *2*-Propenyl sorbate
876 *2*-Propenyl sulfide
745 *2*-Propenyl-*4,6,6*-trimethyl-*1,3*-dioxane
101 *2*-Propenyl undecenoate
102 *2*-Propenyl-*iso*-valerate
2027 *4*-Propenyl veratrole
2643 Propiolic alcohol
2652 .... Propionaldehyde
2653 .... Propione
2654 .... Propionic acid
1344 Propionic ether
2656 Propionyl benzene
2655 .... *2*-Propionyl cyclopentanone
2210 *N*-Propionyl methylanthranilate
2656 .... Propiophenone
1224 *2*-Propoxy-ethanol
2304 *2*-Propoxy naphthalene
233 *3*-Propoxy octene-*1*
9 *n*-Propyl acetal
2657 .... *n*-Propyl acetate
2658 .... *iso*-Propyl acetate
3056 *n*-Propyl acetic acid
3057 *iso*-Propyl acetic acid
1933 *iso*-Propyl acetone
17 *para-iso*-Propyl acetophenone
17 *para-iso*-Propyl acetylbenzol
2737 *para-n*-Propyl-*1*-acetylphenol
1599 *beta*-Propyl acrolein
1603 *beta*-Propyl acrylic acid
2659 .... *iso*-Propyl adipate
2660 .... *n*-Propyl alcohol
2661 .... *iso*-Propyl alcohol
2661 *secondary*-Propyl alcohol
2652 "Propyl aldehyde"
1606 *gamma*-Propyl allylalcohol
2664 *n*-Propyl-*ortho*-aminobenzoate
2664 *iso*-Propyl-*ortho*-aminobenzoate
2041 *iso*-Propyl-*secondary*-amylacetate
2662 .... *n*-Propyl anisate
2663 .... *iso*-Propyl anisate
924 *para-n*-Propyl anisole
2664 .... *n*-Propyl anthranilate
753 *para-iso*-Propyl benzaldehyde
2665 .... Propyl benzene
750 *iso*-Propyl benzene
2666 .... *n*-Propyl benzoate
2667 .... *iso*-Propyl benzoate
756 *para-iso*-Propyl benzoic acid
2665 *n*-Propyl benzol
757 *para-iso*-Propyl benzyl acetate
990 *alpha-iso*-Propyl benzylalcohol
752 *para-iso*-Propyl benzylalcohol
2668 .... *para-iso*-Propyl benzyl butyraldehyde
2669 .... *n*-Propyl benzyl carbinol
2670 .... *iso*-Propyl benzyl carbinol
2671 .... *iso*-Propyl benzyl carbinyl acetate

2672 .... *para-iso*-Propyl benzyl dimethylcarbinol
2673 .... *n*-Propyl benzylether
2674 .... *iso*-Propyl benzylether
2673 *n*-Propyl benzyl oxide
2674 *iso*-Propyl benzyl oxide
2675 .... *iso*-Propyl-*2*-bornanyl ether
2676 *n*-Propyl butanoate
1151 *2-iso*-Propylbutanol pyruvate
2676 .... *n*-Propyl butyrate
2677 .... *n*-Propyl-*iso*-butyrate
2678 .... *iso*-Propyl butyrate
2678 *iso*-Propyl-*n*-butyrate
2679 .... *iso*-Propyl-*iso*-butyrate
2680 .... *alpha*-Propyl-*gamma*-butyrolactone
1504 *gamma-n*-Propyl-*gamma*-butyrolactone
2681 *n*-Propyl caprate
2681 .... *iso*-Propyl caprate
2681 (*iso*)-Propyl caprinate
2682 .... *n*-Propyl caproate
2683 .... *iso*-Propyl caproate
2684 .... *n*-Propyl caprylate
2685 .... *iso*-Propyl caprylate
389 *n*-Propyl carbinol
390 *iso*-Propyl carbinol
2704 *para*-Propylcatechol ethylether
1224 Propyl cellosolve
2688 *n*-Propyl cinnamal
2689 *iso*-Propyl cinnamal
2686 .... *n*-Propyl cinnamate
2687 .... *iso*-Propyl cinnamate
2688 .... *alpha-n*-Propyl cinnamic aldehyde
2689 .... *alpha-iso*-Propyl cinnamic aldehyde
573 *iso*-Propyl-*ortho*-cresol
2944 *3-para-iso*-Propyl-*meta*-cresol
2946 *para-iso*-Propyl-*meta*-cresol ethylether
2947 *para-iso*-Propyl-*meta*-cresol methylether
2690 .... *para-iso*-Propyl cyclohexane ethanol
2691 .... *cis-para-iso*-Propyl cyclohexane propanol
2692 .... *4-iso*-Propyl cyclohexanol
2693 .... *para-iso*-Propyl cyclohexanyl acetate
2458 *4-iso*-Propyl-*1*-cyclohexen-*1*-al
2694 .... *para-iso*-Propyl-*1*-cyclohexenone
2690 *para-iso*-Propyl cyclohexyl ethylalcohol
2691 *3*-(*4-iso*-Propylcyclohexyl)-propan-*1*-ol
2681 (*iso*)-Propyl decanoate
2681 (*iso*)-Propyl decylate
1054 *2-iso*-Propyl-*4,5*-dimethylphenol
2695 .... *1*-Propyl disulfide
1575 *2*-Propylene acrolein
2696 .... Propylene glycol
2697 .... Propylene glycol alginate
2698 .... Propylene glycol diacetate
2699 .... Propylene glycol di-*iso*-butyrate
2700 .... Propylene glycol dipropionate
2701 .... Propylene glycol monoacetate
2702 Propylene glycol mono-octadecanoate
2469 *1,3*-Propyleneglycol monophenylether, *n*-butyrate
2702 Propylene glycol monostearate
2702 .... Propylene glycol stearate
2814 *4*-Propylene-*1,2*-methylenedioxybenzene
2703 .... *iso*-Propyl ether
2732 *para-n*-Propyl ethoxyphenol
2732 *para-iso*-Propyl ethoxyphenol
2704 .... *5*-Propyl-*2*-ethoxyphenol
2705 .... *n*-Propyl formate
2706 .... *iso*-Propyl formate
550 *iso*-Propyl formic acid
2707 .... Propyl-*2*-furanacrylate
2708 .... *alpha-iso*-Propyl furfuracrolein
2709 .... *n*-Propyl furoate
2707 Propyl-*3*-(*2*-furyl)-acrylate
2708 *2-iso*-Propyl-*3*-(*2*-furyl)-*2*-propen-*1*-al
2710 .... *n*-Propyl gallate
944 *n*-Propyl guaiacol
2711 *n*-Propyl heptanoate
2712 *iso*-Propyl heptanoate
2716 *iso*-Propyl heptincarbonate
2711 .... *n*-Propyl heptoate
2712 .... *iso*-Propyl-*n*-heptoate
2711 *n*-Propyl heptylate
2712 *iso*-Propyl heptylate
2713 .... Propyl heptyl ether
2714 .... *iso*-Propyl heptylether
2715 .... *n*-Propyl heptyl ketone
2716 .... *iso*-Propyl-*n*-hept-*1*-yne carbonate
2729 *iso*-Propyl hexadecanoate
2690 *para-iso*-Propyl hexahydrophenylethyl alcohol
2682 *n*-Propyl hexanoate
2683 *iso*-Propyl hexanoate
2682 *n*-Propyl hexoate
2683 *iso*-Propyl hexoate
2682 *n*-Propyl hexylate
2683 *iso*-Propyl hexylate
2717 *para-iso*-Propyl hydratropal
2717 .... *para-iso*-Propyl hydratropic aldehyde
2741 *para-iso*-Propyl hydrocinnamic aldehyde
2000 *para-n*-Propylhydroquinone dimethylether
2748 *n*-Propyl-*ortho*-hydroxybenzoate
2749 *iso*-Propyl-*ortho*-hydroxybenzoate
2718 .... Propyl-*para*-hydroxybenzoate
474 *2*-Propyl-*4*-hydroxymethyl-*1,3*-dioxolane
2660 Propylic alcohol
1856 *iso*-Propylidene acetone
2719 .... *iso*-Propylidene-*3*-acetyl-*1*-cyclopentene-*5*
2719 *3-iso*-Propylidene-*1*-acetylcyclopent-*5*-ene
1505 *cis-n*-Propylidene butyraldehyde
1507 *trans-n*-Propylidene butyraldehyde
1468 *1,2-iso*-Propylidene glycerol
1770 *iso*-Propylidene ionone
2720 .... *3*-Propylidene phthalide
2721 .... *beta-n*-Propyl indole
2722 .... *beta-iso*-Propyl indole
766 *iso*-Propyl ionone
1091 Propyl malonate
2723 .... *n*-Propyl mercaptan

2705 *n*-Propyl methanoate
2706 *iso*-Propyl methanoate
2662 *n*-Propyl-*para*-methoxybenzoate
2663 *iso*-Propyl-*para*-methoxybenzoate
924 *para*-Propyl methoxybenzol
944 *1*-Propyl-*3*-methoxy-*4*-hydroxybenzene
1073 *5-iso*-Propyl-*3*-methoxypyrogallol
2211 *5-iso*-Propyl-*2*-methylacetophenone
2758 *n*-Propyl-*beta*-methylbutyrate
2760 *iso*-Propyl-*beta*-methylbutyrate
2459 *1-iso*-Propyl-*4*-methyl-*2,4*-cyclohexadiene
2459 *4-iso*-Propyl-*1*-methyl-*1,5*-cyclohexadiene
2724 .... *para-iso*-Propyl-*beta*-methylcyclohexane ethanol
1843 *4-iso*-Propyl-*1*-methylcyclohexan-*3*-one
2460 *3-iso*-Propyl-*6*-methylene-*2*-cyclohexene
1837 *d-4-iso*-Propyl-*1*-methyl-*3*-cyclohexene
2909 *2-iso*-Propyl-*5*-methylhexanol-*1*
2910 *2-iso*-Propyl-*5*-methylhexan-*1*-yl acetate
2911 *2-iso*-Propyl-*5*-methylhexan-*1*-yl-*n*-butanoate
2912 *2-iso*-Propyl-*5*-methylhexan-*1*-yl-*iso*-butanoate
2725 .... *para-n*-Propyl methylhydrocinnamic aldehyde
2226 Propyl methyl ketone
2227 *iso*-Propyl methyl ketone
2717 *para-iso*-Propyl-*alpha*-methyl phenylacetaldehyde
2725 *para-n*-Propyl-*alpha*-methyl phenylpropionic aldehyde
2220 *para-iso*-Propyl-*alpha*-methyl phenylpropylalcohol
2677 *n*-Propyl-*2*-methylpropanoate
2679 *iso*-Propyl-*2*-methylpropanoate
2213 *3*-(*para-iso*-Propyl)-*2*-methyl-*2*-propenal
387 "*alpha-iso*-Propyl muguetton"
2726 .... *iso*-Propyl myristate
2304 *n*-Propyl-*beta*-naphthylether
2730 *n*-Propyl nonanoate
2731 *iso*-Propyl nonanoate
2730 *n*-Propyl nonylate
2731 *iso*-Propyl nonylate
2727 *n*-Propyl-*n*-nonynoate
2728 *iso*-Propyl-*n*-nonynoate
2684 *n*-Propyl octanoate
2685 *iso*-Propyl octanoate
2727 *n*-Propyl octin carbonate
2728 *iso*-Propyl octin carbonate
2684 *n*-Propyl octoate
2685 *iso*-Propyl octoate
2684 *n*-Propyl octylate
2685 *iso*-Propyl octylate
2727 .... *n*-Propyl-*n*-oct-*1*-yne carbonate
2728 .... *iso*-Propyl-*n*-oct-*1*-yne carbonate
2716 *iso*-Propyl octynoate
2711 *n*-Propyl oenanthate
2712 *iso*-Propyl oenanthate
2729 .... *iso*-Propyl palmitate
2718 "Propyl paraben"
2718 "Propyl parasept"
2730 .... *n*-Propyl pelargonate
2731 .... *iso*-Propyl pelargonate
2757 *n*-Propyl-*n*-pentanoate
2759 *iso*-Propyl-*n*-pentanoate
2760 *iso*-Propyl-*iso*-pentanoate
2732 *para-n*-Propyl phenethole
2732 .... *para-iso*-Propyl phenethole
2198 *iso*-Propyl phenethyl carbinol
2737 *para-n*-Propyl phenol
2733 .... *para-iso*-Propyl phenol
2173 *alpha-iso*-Propyl phenylacetaldehyde
2734 .... *para-iso*-Propyl phenylacetaldehyde
2735 .... *n*-Propyl phenylacetate
2736 .... *iso*-Propyl phenylacetate
2737 .... *para-n*-Propyl phenyl acetate
751 *para-iso*-Propyl phenylacetic acid
2738 .... *para-iso*-Propyl phenylbutanol
2446 *p*-(*para-iso*-Propylphenyl)-*3*-butanone
2738 *2ara-iso*-Propyl phenyl butyl alcohol
990 *iso*-Propyl phenyl carbinol
12 *n*-Propyl phenylethyl acetal
2671 *alpha-iso*-Propyl phenylethyl acetate
2669 *alpha-n*-Propyl phenylethyl alcohol
2670 *alpha-iso*-Propyl phenylethyl alcohol
2739 .... *beta-para-iso*-Propyl phenylethyl alcohol
2198 *iso*-Propyl phenylethyl carbinol
2740 .... Propyl phenylethyl ether
2446 *para-iso*-Propyl phenylethyl methyl ketone
553 *n*-Propyl phenyl ketone
2220 *3*-(*4-iso*-Propylphenyl)-*2*-methylpropanol
2672 *3*-(*para-iso*-Propylphenyl)-*2*-methylpropan-*2*-ol
2668 *5*-(*para-iso*-Propylphenyl)-pentanal-*1*
2741 *3*-(*para-iso*-Propylphenyl)-propanal-*1*
2741 .... *3*-(*para-iso*-Propylphenyl)-propionic aldehyde
2717 *para-iso*-Propyl-*alpha*-phenylpropionic aldehyde.
2744 *3*-(*para-iso*-Propylphenyl)-*2-iso*-propyl-*2*-propen-*1*-al
2745 *alpha*-Propyl piperidine
2742 *n*-Propyl propanoate
2743 *iso*-Propyl propanoate
2742 .... *n*-Propyl propionate
2743 .... *iso*-Propyl propionate
2744 .... *alpha-iso*-Propyl-*para-iso*-Propyl cinnamic aldehyde
2745 .... *2-n*-Propyl pyridine
2745 *alpha-n*-Propyl pyridine
2746 .... *gamma-n*-Propyl pyridine
2746 *4-n*-Propyl pyridine
2709 *n*-Propyl pyromucate
2747 (*para*)-*iso*-Propyl quinoline
2747 .... *6-iso*-Propyl quinoline
2748 .... *n*-Propyl salicylate
2749 .... *iso*-Propyl salicylate
2750 .... *iso*-Propyl sebacinate
1096 *n*-Propyl succinate

2726 *iso*-Propyl tetradecanoate
2938 Propyl thioaldehyde sulfoxide
2735 *n*-Propyl-*alpha*-toluate
2736 *iso*-Propyl-*alpha*-toluate
819 *para-iso*-Propyl toluene
751 *para-iso*-Propyl-*alpha*-toluic acid
2751 *n*-Propyl-*ortho*-Toluidine
2751 .... *n*-Propyl-*para*-toluidine
2752 *n*-Propyl-*2,2,4*-trimethyl levulinate
2752 .... *n*-Propyl-*2,2,4*-trimethyl-*3*-oxovalerate
2753 .... *1*-Propyl trisulfide
2754 *n*-Propyl undecanoate
2755 *n*-Propyl undecenoate
2756 *iso*-Propyl undecenoate
2754 .... Propyl undecylate
2755 .... *n*-Propyl undecylenate
2756 .... *iso*-Propyl undecylenate
2757 .... *n*-Propyl-*n*-valerate
2758 .... *n*-Propyl-*iso*-valerate
2759 .... *iso*-Propyl-*n*-valerate
2760 .... *iso*-Propyl-*iso*-valerate
2757 *n*-Propyl valerianate
2759 *iso*-Propyl valerianate
2760 *iso*-Propyl-*iso*-valerianate
1054 *5-iso*-Propyl-*meta-4*-xylenol
2643 *2*-Propyn-*1*-ol
1363 Protethyl
2761 .... Protocatechu aldehyde
103 Protocatechu aldehyde-*3*-allylether
3077 Protocatechu aldehyde dimethylether
1363 Protocatechu aldehyde-*3*-ethylether
1484 Protocatechu aldehyde methylene ether
3067 Protocatechu aldehyde methylether
1365 Protocatechu aldehyde methyl ethyl ether
1364 Protocatechu aldehyde-*para*-monoethyl ether
2761 Protocatechuic aldehyde
572 Provitamin A
2350 "Prunolide"
1713 "Prussic acid"
698 Pseudo allyl-*alpha*-ionone
405 Pseudo butyl benzene
1169 Pseudo hexyl acetate
2762 .... Pseudo ionone
2763 .... Pseudo linalyl acetate (see also 2285)
2764 .... Pseudo methyl ethyl ionone
2765 .... Pseudo methyl ionone
2766 .... Pseudo-*iso*-methyl ionone
2765 Pseudo-*normal*-methyl ionone
3021 Pseudo umbellulone
2767 .... Pulegol
2768 .... *iso*-Pulegol
2768 *dextro-iso*-Pulegol
2768 *dextro-neo*-Pulegol
2768 *dextro-neo-iso*-Pulegol
2768 *laevo-iso*-Pulegol
2769 .... Pulegone
2770 .... *iso*-Pulegone
2771 .... *iso*-Pulegyl acetate (see also 663)
2772 .... *iso*-Pulegyl acetoacetate
2773 .... *iso*-Pulegyl-*iso*-butyrate
2774 .... *iso*-Pulegyl formate
2775 .... Pyrazine
1187 Pyrethronic acid, ethylester
2776 .... Pyridine
2777 Pyridine-*2*-aldehyde
499 *beta*-Pyridine carboxylic acid, *n*-butylester
499 *3*-Pyridine carboxylic acid, *n*-butylester
2126 *3*-Pyridine carboxylic acid, methyl ester
2777 .... Pyridyl-*2*-methanal
Pyrocatechin ... see also: Pyrocatechol ....
883 Pyrocatechin di-*n*-butyl ketal
884 Pyrocatechin di-*iso*-butyl ketal
588 Pyrocatechin diethyl ether
3078 Pyrocatechin dimethyl ether
589 Pyrocatechin di-*n*-propyl ketal
590 Pyrocatechin di-*iso*-propyl ketal
1927 Pyrocatechin methyl-*n*-butyl ketal
592 Pyrocatechin methyl hexyl ketal
1901 Pyrocatechol methyl amyl ketal
1927 Pyrocatechol methyl butyl ketal
591 Pyrocatechol monomethylene ether
2778 .... Pyrogallol dimethylether
2779 Pyrogallol-*1*-ethylether
2779 .... Pyrogallol monoethyl ether
2780 .... Pyroligneous acid
2780 Pyroligneous acid extract
2780 Pyroligneous vinegar
1418 Pyromucic acid
83 Pyromucic acid, allyl ester
178 Pyromucic acid, *n*-amylester
1664 Pyromicic acid, *n*-hexylester
1413 Pyromucic aldehyde
1419 Pyromucyl acetone
2781 .... *alpha*-Pyrone
2782 .... *gamma*-Pyrone
2781 *1,2*-Pyrone
2782 *1,4*-Pyrone
2785 Pyroracemic acid
865 Pyroracemic acid, decylester
2783 .... Pyrrole
2784 .... Pyrrolidine
2786 Pyruvaldehyde
35 Pyruvic acetate
2785 .... Pyruvic acid
217 Pyruvic acid, *iso*-amylester
34 Pyruvic alcohol
2786 .... Pyruvic aldehyde

**Q**

2854 "Quadrofos"
1363 "Quatrovanil"
2835 Quillayabark
1748 Quinacetophenone-*5*-methylether
2234 Quinaldine
2787 .... Quinine
2788 .... Quinine bisulfate
2789 Quinine chloride
2789 .... Quinine hydrochloride
2789 Quinine monohydrochloride
2790 .... Quinine sulfate
1717 Quinol

1718 Quinol diethylether
1719 Quinol dimethylether
2791 .... Quinoline
2792 .... *iso*-Quinoline
1720 Quinol methyl ethyl ether
1721 Quinol monoethyl ether
1722 Quinol monomethyl ether
282 *para*-Quinone

**R**

1220 "Radisol"
2087 "Raldeine beta"
2088 "Raldeine delta"
2086 "Raldeine gamma"
1760 "Rasketone"
1307 "Raspberry aldehyde" (so-called)
1760 "Raspberry ketone"
248 "Raspberry ketone methylether"
2553 Redol
1747 Resacetophenone-*4*-methylether
2553 Resedal
2553 Resedalia
2553 Resedol
1197 "Resedone" (see also 1969)
2553 Resedozon
2255 Resocyanin
2013 Resocyanin ethylether
2256 Resocyanin methylether
2793 Resorcin
2793 .... Resorcinol
2794 .... Resorcinol decamethylene ether
2795 .... Resorcinol diacetate
2794 Resorcinol di-*iso*-amyl ketal
2796 .... Resorcinol dimethylether
2795 Resorcinol monoacetate
1057 *beta*-Resorcylaldehyde dimethylether
2162 "Reyn-o-miral"
57 *4*-Rhodan benzaldehyde
495 "Rhodial"
1363 Rhodiarome
658 "Rhodinal"
210 "Rhodinax"
2797 .... Rhodinol (see also 670)
2797 Rhodinol C
2797 Rhodinol coeur
666 "Rhodinolic acid"
2798 .... Rhodinyl acetate
2799 .... Rhodinyl benzoate
2800 .... Rhodinyl-*n*-butyrate
2801 .... Rhodinyl-*iso*-butyrate
2802 .... Rhodinyl cinnamate
2803 .... Rhodinyl formate
2808 Rhodinyl-*beta*-methylbutyrate
688 Rhodinyl oxyacetaldehyde
2807 Rhodinyl pentanoate
2804 .... Rhodinyl phenylacetate (see also 690)
2805 .... Rhodinyl propionate
2806 .... Rhodinyl salicylate
2807 .... Rhodinyl-*n*-valerate
2808 .... Rhodinyl-*iso*-valerate
2807 Rhodinyl valerianate
2808 Rhodinyl-*iso*-valerianate
2088 Rhodione methyl delta
1035 "Rhodisol"
1097 Ribotide (see also 1098)
2273 "RL-50"
2976 "Rodalin"
2976 "Rosacetol"
844 "Rosal" (see also 2485)
844 "Rosalva"
2976 "Rosamen"
2976 "Rosatol"
846 "Roseate"
2809 .... Rose oxide (see also 409)
2976 "Rosephenone"
2976 "Rose solide"
2976 "Rosetone"
2977 "Rosetone"-*n*-butyrate
2978 "Rosetone" propionate
1032 "Rosidol"
2976 "Rosindol"
2676 "Rosone"
2976 "Rosonone"
1032 "Rosorcol"
2140 "Rue ketone"
1324 Rum ether
1258 "Rutgers 6-12"

**S**

2810 .... Sabinene
2811 .... Sabinol
2812 .... Saccharin
561 Saccharin calcium
2857 Saccharin, sodium salt
869 Safranal
2813 .... Safrole
2814 .... *iso*-Safrole
2836 Sage, sclary (Sauge sclarée)
1832 Sake (Japanese rice wine)
1350 "Sal ethyl"
2815 Salicylaldehyde
1864 Salicylaldehyde methylether
1266 Salicylic acid, *2*-ethylhexanoic est
1878 Salicylic acid, methoxymethyleste
2815 .... Salicylic aldehyde
1350 "Salicylic ether
1095 Salicylalcohol di-*iso*-propyl ketal
114 "Salmiac"
2607 Salol
2851 Salt
113 Salt, smelling
2819 Sandalwood oil (see also 2820)
2816 .... Santalal
2816 Santalaldehyde
2817 .... *alpha*-Santalene
2818 .... *beta*-Santalene
2819 .... *alpha*-Santalol
2820 .... *beta*-Santalol
827 "Santalozon"
2821 .... Santalyl acetate
2822 .... Santalyl anthranilate
2823 .... Santalyl benzoate
2824 .... Santalyl-*n*-butyrate
2825 .... Santalyl-*iso*-butyrate
2826 .... Santalyl cinnamate
2827 .... Santalyl formate
2830 Santalyl-*ortho*-hydrobenzoate
2832 Santalyl-*beta*-methylbutyrate
2831 Santalyl-*n*-pentanoate
2828 .... Santalyl phenylacetate
2829 .... Santalyl propionate
2830 .... Santalyl salicylate

2831 .... Santalyl-*n*-valerate
2832 .... Santalyl-*iso*-valerate
2833 .... Santene
2834 .... Santenone
827 "Santiat"
2835 Sapogenin
2835 .... Saponin
2835 Sarsaparilla
2813 Sassafras oil
2810 Savin oil (see also 2811)
2836 .... Sclareol
2837 .... Sebacic acid
914 "Sebacyl ether"
2838 Sedanoic acid, anhydride (= enol-lactone)
2838 .... Sedanoic anhydride
2839 .... Sedanolic acid
2840 Sedanolic acid, lactone
2840 .... Sedanolide (see also 517)
2841 .... Sedanonic acid
2842 .... *alpha*-Selinene
2843 .... *beta*-Selinene
1367 "Selinenol"
2844 .... Serine
2845 .... Shogaol
353 "Siberian Pine needle oil, terpeneless" (so-called)
1062 Silveterpineols
1742 Sinapyl alcohol
1027 "Sinensal"
2860 "Sionon"
2846 .... Skatole
2082 "*iso*-Skatole"
2847 .... Skatolene
2847 Skatole-hydroxycitronellal ("Schiff's base")
3020 Skimmetin
113 "Smelling salt"
2780 "Smoke, liquid"
2835 Soap plant, Californian
2625 Sobrerene dihydrate
2625 Sobrerol
2855 Soda, caustic
2848 .... Sodium acetate
2850 Sodium acid carbonate
2849 .... Sodium benzoate
2857 Sodium-*ortho*-benzosulfimide
2850 .... Sodium bicarbonate
2851 .... Sodium chloride
2852 .... Sodium citrate
2853 .... Sodium cyclamate
2853 Sodium cyclohexane sulfamate
2854 Sodium gluconate
2854 .... Sodium hexametaphosphate
2855 Sodium hydrate
2850 Sodium hydrogen carbonate
2855 .... Sodium hydroxide
2854 Sodium metaphosphates
2856 .... Sodium-*ortho*-methyl cyclohexyl sulfamate
2857 .... Sodium saccharin
2854 Sodium tartrate
2854 Sodium thiosulfate
1468 "Solketal"
2857 Soluble saccharin
1051 Solvarom
913 Solveol
2858 .... Sorbic acid
1577 Sorbic alcohol
1575 Sorbic aldehyde
2859 .... Sorbitan monostearate
2860 *dextro*-Sorbite
2860 .... Sorbitol
2860 "Sorbo"
559 "Sorbo-calcion"
2860 *dextro*-Sorbol
1577 Sorbyl alcohol
1578 Sorbyl-*iso*-butyrate
2858 Sorbus aucuparia
2859 "Span" (see also 2635)
2028 "Sparassol"
341 Spasmin
292 Spasmodin
2861 .... *laevo*-Spicatone
1311 "Spirit of Nitrous ether"
2012 "Spirosal"
537 "Spoonwort oil, artificial"
538 "Spoonwort oil, true"
2862 .... Squalene
2863 .... Stearic acid
2391 Stearaldehyde
2391 Stearic aldehyde
1117 "Stearolactone"
2392 "Stenol"
2864 .... Stilbene
2864 *cis*-Stilbene
2864 *iso*-Stilbene
1728 "Storine"
1306 "Strawberry aldehyde"
633 "Styracine"
2176 Styrallyl acetate
2175 Styrallyl alcohol (see also 2563)
2177 Styrallyl anthranilate
2178 Styrallyl benzoate
2179 Styrallyl butyrate
2180 Styrallyl-*iso*-butyrate
2181 Styrallyl caproate
2183 Styrallyl cinnamate
2184 Styrallyl formate
2182 Styrallyl octylate
2185 Styrallyl phenylacetate
2186 Styrallyl propionate
2187 Styrallyl salicylate
2188 Styrallyl-*iso*-valerianate
2865 .... Styrene
2563 Styrene glycol
11 Styrene glycol acetal
2866 .... Styrene oxide
2865 "Styrol"
2865 Styrolene
2176 "Styrolene acetate"
2568 "Styrolyl acetate I"
2569 "Styrolyl acetate II"
2563 "Styrolyl alcohol" (see also 2175)
2564 "Styrolyl anthranilate"
2570 "Styrolyl benzoate"
2566 "Styrolyl diacetate"
2567 "Styrolyl formate"
2574 "Styrolyl-*primary*-mono-phenylacetate"

2572 “Styrolyl propionate I”
618 “Styrone”
2495 “*iso*-Styrone”
2495 “*iso*-Styrone acetate”
2608 Styryl acetate
371 Styryl bromide
618 Styryl carbinol
641 Styryl cyanide
623 *2*-Styryl-*1,3*-dioxolane
621 *2*-Styryl-*4,4,6*-trimethyl-*1,3*-dioxan
560 “Sucaryl”
560 “Sucaryl calcium”
2853 “Sucaryl sodium”
2867 .... Succinic acid
116 “Sucramine”
1125 “Sucrol”
2868 .... Sucrose octa-acetate
2812 *ortho*-Sulfobenzimide
2869 .... Sulfur dioxide
2869 Sulfurous anhydride
2869 Sulfurous oxide
906 Sulfuric ether
1363 “Supervanil”
989 “Surolene”
471 “Sustane”
2870 .... Sylvestrene
2191 “Syringa alcohol”
2189 “Syringa alcohol, acetate”
2954 Syringa aldehyde
1742 Syringic aldehyde
2954 Sylvanal (see also 1696)

**T**

533 “Tabutrex”
1343 Tagetol
2940 Tanacetone
2941 Tanacetyl alcohol
2871 .... Tannic acid
2871 Tannin
2296 “Tar camphor”
2872 .... Tartaric acid
2980 T.C.P.
2241 “Teaberry oil, synthetic”
1717 Tecquinol
470 “Tegosept B”
2718 “Tegosept gamma”
469 “Tenox BHA”
471 “Tenox BHT”
2710 “Tenox PG”
1935 “Tepyl acetate” (see also 2346)
2882 “Tereben”
1836 Terpane
2873 .... *alpha*-Terpinene
2874 .... *gamma*-Terpinene
2875 .... *1*-Terpinenol
2876 .... *4*-Terpinenol
2877 .... *alpha*-Terpineol
2878 .... *beta*-Terpineol
2879 .... *gamma*-Terpineol
2880 .... Terpin hydrate
2881 .... Terpinol
2882 .... Terpinolene
2883 .... Terpinyl acetate
2884 .... Terpinyl anthranilate
2885 .... Terpinyl benzoate
2886 .... Terpinyl-*n*-butyrate
2887 .... Terpinyl-*iso*-butyrate
2888 .... Terpinyl cinnamate
2889 .... Terpinyl formate
2890 .... Terpinyl phenylacetate
2891 .... Terpinyl propionate
2892 .... Terpinyl-*n*-valerate
2893 .... Terpinyl-*iso*-valerate
854 *gamma*-Tetradecalactone
2894 Tetradecamethylene carbonate
2894 .... Tetradecamethylene carboxylate
2290 Tetradecanal
2261 *iso*-Tetradecanal
2288 Tetradecanoic acid
2289 *1*-Tetradecanol
853 *alpha*-Tetradecanolide-*1:4*
2290 Tetradecyl aldehyde
2292 Tetradecyl nitrile
2 Tetrahydro abietyl alcohol
37 Tetrahydro acetophenone
2918 Tetrahydro allo-ocimenol
2919 Tetrahydro allo-ocimenylacetate
374 *1,2,5,6*-Tetrahydro-*3*-(buten-*2*-yl)-benzaldehyde
375 *1,2,3,5*-Tetrahydro-*3*-(buten-*2*-yl)-benzylalcohol
2838 Δ*12*-Tetrahydro-*n*-butylidene phthalide
2840 Δ*13*-Tetrahydro-*n*-butyl phthalide
2895 .... Tetrahydro-*iso*-butylquinoline
2896 .... Tetrahydro cinnamic aldehyde
2458 Tetrahydro cuminaldehyde
1062 Tetrahydro dimethyl benzyl carbinol
2923 Tetrahydro ethyltetralol
2897 .... Tetrahydro farnesal
2898 .... Tetrahydro furan
2900 Tetrahydro-*3*-furancarbinol
2906 Tetrahydro furanethylalcohol
2900 Tetrahydro-*3*-furanmethanol
2899 .... Tetrahydro furfuryl acetate
2900 .... Tetrahydro furfuryl alcohol
2901 .... Tetrahydro furfuryl-*n*-butyrate
2902 .... Tetrahydro furfuryl cinnamate
2903 .... Tetrahydro furfuryl crotonate
2904 .... Tetrahydro furfuryl phenylacetate
2905 .... Tetrahydro furfuryl propionate
2906 .... *2*-(Tetrahydrofuryl)-ethanol-*2*
2900 Tetrahydro-*2*-furylmethanol
2899 Tetrahydro-*2*-furyl methylacetate
2901 Tetrahydro-*2*-furyl methyl-*n*-butanoate
2903 Tetrahydro-*2*-furyl methyl-*2*-butenoate
2902 Tetrahydro-*2*-furyl methyl cinnamate
2903 Tetrahydro-*2*-furyl methyl-*alpha*-crotonate
2905 Tetrahydro-*2*-furyl methyl propionate
2904 Tetrahydro-*2*-furyl methyl-*alpha*-toluate
1031 “Tetrahydro geranial” (see also 931)
1032 Tetrahydro geraniol
1033 Tetrahydro geranyl acetate
1034 Tetrahydro geranyl phenylacetate
1582 Tetrahydro-*6*-hydroxy dicyclopentadiene
2907 .... Tetrahydro ionone

2908 .... Tetrahydro jasmone (see also 1533 and 1903)
2909 .... Tetrahydro lavandulol
2910 .... Tetrahydro lavandulyl acetate
2911 .... Tetrahydro lavandulyl-*n*-butyrate
2912 .... Tetrahydro lavandulyl-*iso*-butyrate
2913 .... Tetrahydro linalool
2914 .... Tetrahydro linalyl acetate
1835 Tetrahydro manool
2915 .... Tetrahydro-*2*-(*para*-menthan-*7*-yl-methoxy)-pyran
1570 Tetrahydro methylabietate
2916 .... *1*-Tetrahydro-$\Delta^1$-*para*-methylacetophenone
1973 Tetrahydro-*para*-methylbenzylidene acetone
2917 .... Tetrahydro-*para*-methylquinoline
1716 Tetrahydro-*2*-methylquinoline
2917 *1,2,3,4*-Tetrahydro-*6*-methylquinoline
2918 .... Tetrahydro muguol
2919 .... Tetrahydro mugyl acetate
2920 .... Tetrahydro myrcenol
2921 .... Tetrahydro-*alpha*-naphthol ethylether
2922 .... *5,6,7,8*-Tetrahydro-*1*-(or-*2*-)-naphthylacetaldehyde
2923 Tetrahydro-*beta*-*1*-naphthyl ethanol
2923 .... Tetrahydro naphthyl ethyl alcohol
3014 Tetrahydro-nor-farnesal
2924 .... Tetrahydro-*2*-(phenethoxy)-pyran
2925 .... Tetrahydro-pseudo-ionone
2929 Tetrahydropyran-*2*-*para*-cresylether
2926 .... Tetrahydro pyranyl crotonate
2346 Tetrahydro pyranylethers
2924 Tetrahydro pyranyl phenylethyl ether
2929 Tetrahydro pyranyl-*2*-tolylether
954 Tetrahydro pyrethrone
2784 Tetrahydro pyrrole
2927 .... Tetrahydro quinoline
3092 Tetrahydro styrene
2917 Tetrahydro-*para*-toluquinone
2928 .... Tetrahydro-*para*-tolylaldehyde
2929 .... Tetrahydro-*2*-(*para*-tolyloxy)-pyran
1804 Tetrahydro-*2,2,6*-trimethyl-*6*-vinylpyran-*3*-ol
2419 *4*-(*2,2,4,4*-Tetramethylbutyl)-cyclohexanone
2240 *2,4,6,6*-Tetramethyl cyclohexa-*1*:*3*-dienal
951 *1*-(*2,5,6,6*-Tetramethyl-*2*-cyclohexenyl)-butan-*3*-one (*cis*- and *trans*-)
2091 *4*-(*2,3,6,6*-Tetramethyl-*3*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
2092 *4*-(*2,4,6,6*-Tetramethyl-*1*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
2092 *4*-(*2,4,6,6*-Tetramethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
1784 *4*-(*2,5,6,6*-Tetramethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
1435 *2,6,9,9*-Tetramethyl-*2,6*-decadienal
1435 *2,2,5,9*-Tetramethyl-*4,8*-decadien-*1*-al
1439 *2,2,5,9*-Tetramethyl-*4,8*-decadiene-*1*-nitrile
1439 *2,6,9,9*-Tetramethyl-*2,6*-decadienoic acid, nitrile
2240 *2,4,6,6*-Tetramethyl-*5,6*-dihydro-benzaldehyde
2898 Tetramethylene oxide
3080 *1,1,4,4*-Tetramethyl-*6*-ethyl-*7*-acetyl-*1,2,3,4*-tetrahydronaphthalene
2930 .... Tetramethyl ethyl cyclohexenone
2616 Tetramethyl ethylene glycol
2617 Tetramethyl ethyleneglycol dimethylether
1449 *3,7,11,15*-Tetramethyl-*1,6,10,14*-hexadecatetraen-*3*-ol
2614 *3,7,11,15*-Tetramethyl-*1*-hexadecen-*3*-ol
2613 *3,7,11,15*-Tetramethyl-*2*-hexadecen-*1*-ol
2615 *3,7,11,15*-Tetramethyl-*2*-hexadecen-*1*-yl acetate
1589 Tetramethyl-*beta*-hexalone
394 *2,2,4,4*-Tetramethylhexan-*3*-one
2931 .... *2,5,5,9*-Tetramethyl-*1*-hydroxy-*1,2,3,5,6,7,8,9*-Octahydronaphthalin
2931 *2,5,5,9*-Tetramethyl-*1,2,3,5,6,7,8,9*-octahydro-*alpha*-naphthol
2932 Tetramethyl octahydro-*alpha*-naphthyl acetaldehyde
2933 Tetramethyl octahydro-*alpha*-naphthyl ethylalcohol
2931 Tetramethyl octalol
2932 .... $\Delta^{2,3}$-(and $\Delta^{1,2}$-)-*2,5,5,9*-tetramethyl octalyl-*1*-ethanal
2933 .... $\Delta^{2,3}$-(and $\Delta^{1,2}$-)-*2,5,5,9*-tetramethyl octalyl-*1*-ethanol
2917 "Tetraquinone"
1412 Tetrole
453 Tetryl formate
558 Theine
2900 T.H.F.A.
811 "Thibetolide"
2934 .... *2*-Thienyl mercaptan
2934 *2*-Thienyl thiol
876 Thioallyl ether
488 *n*-Thiobutyl alcohol
57 *para*-Thiocarbimide benzaldehyde
2935 .... Thioglycollic acid
2936 .... Thioguaiacol
2937 .... Thiophenol
2938 .... Thiopropanal-*S*-oxide
2723 *n*-Thiopropyl alcohol
2952 *beta*-Thiotolene
57 "Thiotrope base"
2939 .... Threonine
2940 .... Thujone
2941 .... Thujyl alcohol
2944 "Thyme camphor"
2942 .... Thymohydroquinone
2943 .... Thymohydroquinone dimethylether
2944 .... Thymol
2945 .... *iso*-Thymol (see also 573)
2944 *meta*-Thymol
2946 .... Thymol ethylether
2947 .... Thymol methylether
2948 .... Thymyl propionate
2949 .... Tiglic acid

2950 .... Tiglic aldehyde
2951 .... Tiglyl piperidide
1728 "Tilleul"
2959 "Tolualdehyde"
2470 *alpha*-Tolualdehyde
2960 *meta*-Tolualdehyde
2961 *ortho*-Tolualdehyde
2962 *para*-Tolualdehyde
2963 Tolualdehyde glycerinacetal
2952 .... Toluene
325 *alpha*-Toluene thiol
2953 .... Toluhydroquinone dimethylether
2492 *alpha*-Toluic acid
2970 *alpha*-Toluic aldehyde
2960 *meta*-Toluic aldehyde
2961 *ortho*-Toluic aldehyde
2962 *para*-Toluic aldehyde
2952 Toluol
2236 *meta*-Toluquinoline
2237 *ortho*-Toluquinoline
2238 *para*-Toluquinoline
2953 "Toluquinone dimethylether"
2864 Toluylene
2654 .... *para*-Tolyl acetaldehyde
1915 *meta*-Tolyl acetate
2955 .... *ortho*-Tolyl acetate
2956 .... *para*-Tolyl acetate
2957 .... *ortho*-Tolyl alcohol
2958 .... *para*-Tolyl alcohol
2959 .... Tolyl aldehyde (mixed isomers: *ortho-meta-para-*)
2470 *alpha*-Tolyl aldehyde
2960 .... *meta*-Tolyl aldehyde
2961 .... *ortho*-Tolyl aldehyde
2962 .... *para*-Tolyl aldehyde
2485 *alpha*-Tolylaldehyde dimethyl acetal
2963 .... Tolylaldehyde glyceryl acetal
1921 Tolylaldehyde propyleneglycol (cyclic) acetal
2964 .... *para*-Tolyl anthranilate
726 *para*-Tolyl benzoate
2965 .... *2*-Tolyl benzothiazole
727 *para*-Tolyl benzoyl acetate
2170 Tolyl benzyl ether
2966 .... *4*-(*para*-Tolyl)-*2*-butanol
2967 .... *4*-(*para*-Tolyl)-*2*-butanone
728 *para*-Tolyl-*n*-butyrate
729 *para*-Tolyl-*iso*-butyrate
2968 .... *alpha*-Tolyl-*gamma*-butyrolactone
2957 *ortho*-Tolylcarbinol
2958 4-Tolyl carbinol
1915 *meta*-Tolylcarbinyl acetate
2003 "*para*-Tolyl"-dimethyl carbinol
2969 *para*-Tolyl dodecanoate
2190 *ortho-2*-Tolylethan-*1*-ol
2191 *para-2*-Tolylethan-*1*-ol
712 *meta*-Tolylether
713 *para*-Tolylether
2189 *2-para*-Tolyl ethylacetate
2191 "Tolyl ethylalcohol"
2963 "Tolyl glycerin"
2969 .... *para*-Tolyl laurate
1595 "Tolyl mercaptal"
nitrile
730 *para*-Tolyl octanoate
730 *para*-Tolyl octoate
2970 .... *para*-Tolyl-*n*-octylketone
737 *meta*-(or *1,3*-)-Tolyl phenylacetate
738 *ortho*-(or *1,2*-)-Tolyl phenylacetate
739 *para*-(or *1,4*-)-Tolyl phenylacetate
1923 *para*-Tolylpropionate
2070 *2*-(*para*-Tolyl)-propionic aldehyde
41 "Tonalid"
934 Toncainol
1965 Toncair
1965 "Toncarine"
704 "Tonka camphor"
1719 "Tonkaine"
1590 "Tonkalide"
934 "Tonkamel"
1965 "Tonkarin"
3017 "Tonquinol"
1828 Toxilic acid
218 "Trefle"
1660 "Treflol"
218 "Trefol"
218 "Tresseine"
2971 .... Triacetin
162 Triamylcitrate
2972 .... Tributyl acetylcitrate
428 Tributyl citrate
2973 .... Tributyrin
2974 .... Tricalcium phosphate
2976 $1^2,1^2,1^2$-Trichloro-$1^1$-acetoxy-*1*-ethylbenzene
609 Trichloro methane
2975 .... Trichloro methyl phenyl carbinol
2976 .... Trichloro methyl phenyl carbinyl acetate
2977 .... Trichloro methyl phenyl carbinyl butyrate
2978 .... Trichloro methyl phenyl carbinyl propionate
2976 Trichloro-*alpha*-phenylethyl acetate
2975 Trichloro-*alpha*-phenylethyl alcohol
2977 Trichloro-*alpha*-phenylethyl-*n*-butanoate
2978 Trichloro-*alpha*-phenylethyl propionate
2975 Trichloro styrallylalcohol
2979 .... Tricholomic acid
2980 .... Tricresyl phosphate
562 Tricyclene
2981 .... Tricyclopentadiene
3081 Tricyclo vetiverol
2982 .... *delta*-Tridecalactone
2984 Tridecaldehyde
2983 Tridecamethylene carbonate
2983 .... Tridecamethylene carboxylate
2984 .... Tridecanal
2141 "*iso*-Tridecanal"
2288 Tridecan carboxylic acid
1214 Tridecane dioic acid, cyclic ethyleneglycol diester
2985 .... Tridecanoic acid
2986 .... Tridecanol-*1*
2982 *delta*-Tridecanolide
2948 .... Thymyl propionate
2949 .... Tiglic acid

2370 Tridecanolide-*1:4*
2262 *2*-Tridecanone
922 Tridecanone-*7*
2987 .... *2*-Tridecenal
2987 Tridecen-*2*-al-*1*
2989 *2*-Trideceen-*1*-ol
2989 Tridecenyl alcohol
2988 .... Tridecyl acetate
2986 Tridecyl alcohol
2984 Tridecyl aldehyde
2292 Tridecyl cyanide
2989 .... Tridecylenic alcohol
2985 Tridecylic acid
1323 Triethoxy methane
1141 Triethyl aconitate
2990 .... Triethyl citrate
2991 .... Triethylene glycol
1072 Trihydroxycinnamic acid, *delta*-lactone
1467 Trihydroxypropane
2992 .... *2,4,6*-Trimethoxy benzoylacetone
3005 Trimethoxy methane
2992 *5*-(*2,4,6*-Trimethoxyphenyl)-pentane-*2,4*-dione
264 *1,2,4*-Trimethoxy-*5*-propenylbenzene
42 *1,3,5*-Trimethyl acetophenone
42 *2,4,6*-Trimethyl acetophenone
2993 .... *2,5,5*-Trimethyl-*2*-amyl-*1,3*-dioxane
2994 Trimethyl benzaldehydes
1855 *1,3,5*(*=symmetric*)-Trimethyl benzene
2994 .... Trimethyl benzonitrile
2483 *4,4,6*-Trimethyl-*2*-benzyl-*1,3*-dioxan
1387 *1,3,3*-Trimethylbicyclo-*1,2,2*-heptanol-*2*
350 *1,7,7*-Trimethylbicyclo-*1,2,2*-heptanol-*2*
2621 *2,6,6*-Trimethylbicyclo-*1,3,3*-heptanol-*3*
1385 *1,3,3*-Trimethylbicyclo-*1,2,2*-heptanone-*2*
565 *1,7,7*-Trimethylbicyclo-(*2,2,1*)-*2*-heptanone
2622 *2,6,6*-Trimethyl-*1,3,3*-bicycloheptanone-*3*
2619 *2,6,6*-Trimethylbicyclo-(*3,1,1*)-*2*-heptene
570 *3,7,7*-Trimethylbicyclo-*0,1,4*-heptene-*3*
2995 .... *1,1,7*-Trimethylbicyclo-(*1,1,3*)-hepten-*1*-one
3079 *2,6,6*-Trimethyl-(*1,3,3*)-bicyclohept-*2*-en-*4*-one
571 *3,7,7*-Trimethyl-(*0.1.4*)-bicyclo-*3*-hepten-*2*-one
392 Trimethyl carbinol
1957 Trimethyl citrate
2996 .... *4*-(*2,6,6*-Trimethyl-*7*-cycloheptenyl)-*3*-buten-*2*-one
869 *2,6,6*-Trimethyl-*4,6*-cyclohexadiene-*1*-carboxaldehyde
2997 .... *alpha*-*2,4*-Trimethyl cyclohexane methylacetate
2998 .... Trimethyl cyclohexanol
967 *3,5,5*-Trimethyl cyclohexanone
2999 .... *3,5,5*-Trimethyl cyclohexanone ethylglycidate
3003 *3,5,5*-Trimethyl cyclohexanyl acetate
3000 .... *2,2,4*-Trimethyl-*3*-cyclohexen-*1*-aldehyde diethylacetal
760 *2,2,6*-Trimethyl-*5*-cyclohexen-*1*-carboxaldehyde
760 *2,2,6*-Trimethyl-*6*-cyclohexen-*1*-carboxaldehyde
761 *2,4,6*-Trimethyl-*4*-cyclohexen-*1*-carboxaldehyde
761 *3,5,6*-Trimethyl-*3*-cyclohexen-*1*-carboxaldehyde
2610 *3,5,5*-Trimethyl-*2*-cyclohexen-*1*-ol
3001 .... *1,1,3*-Trimethyl-*2*-cyclohexenone-*4*
3001 *2,4,4*-Trimethyl-*2*-cyclohexen-*1*-one
2611 *3,5,5*-Trimethyl-*2*-cyclohexen-*1*-one
764 *beta*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-acrylonitrile
949 *4*-(*2,6,6*-Trimethyl cyclohexen-*1*-yl)-butan-*2*-one
869 *4*-(*2,2,6*-Trimethyl-*1*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
1777 *4*-(*2,2,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
3002 .... *4*-(*2,4,6*-Trimethyl-*3*-cyclohexen-*1*-yl)-*3*-buten-*2*-one
3011 *4*-(*2,6,6*-Trimethyl-*4*-cyclohexenyl)-*3* buten-*2*-one
2084 *4*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-*2,3*-dimethyl-*2*-buten-*1*-al
86 *1*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*1,6*-heptadien-*3*-one
1274 *6*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*5*-hexen-*4*-one
2086 *4*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*3*-methyl-*3*-buten-*2*-one
2088 *4*-(*2,6,6*-Trimethyl-*3*-cyclohexen-*1*-yl)-*3*-methyl-*3*-buten-*2*-one
1770 *6*-(*2,6,6*-Trimethyl-*1*-(or-*3*)-cyclohexen-*1*-yl)-*1*-methyl-*2,5*-hexadien-*4*-one
766 *6*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*1*-methyl-*5*-hexen-*4*-one
765 *5*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*4*-methyl-*4*-penten-*3*-one
961 *5*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-pentan-*3*-one
2087 *5*-(*2,6,6*-Trimethyl-*1*-cyclohexen-*1*-yl)-*4*-penten-*3*-one
2085 *5*-(*2,6,6*-Trimethyl-*2*-cyclohexen-*1*-yl)-*4*-penten-*3*-one
572 *1,18-bis*-(*2,6,6*-Trimethylcyclohexen-*6*-yl)-*3,7,13,16*-tetramethyl octadecanonaene
764 *beta*-(*2,6,6*-Trimethyl-*2*-cyclohexenyl)-vinylcyanide
3003 .... Trimethyl cyclohexyl acetate
2907 *4*-(*2,6,6*-Trimethyl cyclohexyl)-butan-*2*-one
947 *2,6,6*-Trimethyl cyclohexyl-*1*-buten-*3*-one
3004 .... *1,1,8*-Trimethyl-*2*-cyclo-octanone
427 *3,7,9*-Trimethyl-*2,6*-decadien-*1*-al
484 *3,7,9*-Trimethyl-*1,6*-decadien-*3*-ol

1065 *1,2,4*-Trimethyl-*3,5*-dinitro-*6*-*tertiary*-butylbenzene
558 *1,3,7*-Trimethyl-*2,6*-dioxypurine
1510 *2,6,10*-Trimethyl dodecanal
2897 *2,6,10*-Trimethyl-*10*-dodecen-*12*-al
2897 *3,7,11*-Trimethyl-*2*-dodecen-*1*-al
1379 *2,6,10*-Trimethyl-*2,6,9,11*-dodecatetraene
1378 *2,6,10*-Trimethyl-*2,6,10*-dodecatrien-*12*-al
1380 *2,6,10*-Trimethyl-*2,6,10*-dodecatrien-*12*-ol
1380 *3,7,11*-Trimethyl-*2,6,10*-dodecatrien-*1*-ol
2316 *3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-ol
2317 *3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl acetate
2318 *3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl-*iso*-butyrate
2319 *3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl formate
2320 *3,7,11*-Trimethyl-*1,6,10*-dodecatrien-*3*-yl propionate
2647 *2,6,7*-Trimethylene-*3*-hydroxy methylheptane
122 Trimethyl ethylacetate
3005 .... Trimethyl-*ortho*-formate
869 *1,1,3*-Trimethyl-*2*-formylcyclohexadien-*2,4*
263 *2,5,5*-Trimethylheptadien-*2,6*-one-*4*
3006 .... *3,5,5*-Trimethyl hexanal
3007 .... Trimethyl hexanol
3008 .... *3,5,5*-Trimethyl hexyl acetate
3007 Trimethyl hexyl alcohol
2931 Trimethyl hydroxyoctahydronaphthalin
108 *2,2,4*-Trimethyl-*2*-hydroxy octalin
2752 *2,2,4*-Trimethyl-*gamma*-ketovaleric acid, *n*-propylester
431 "*2,4,6*-Trimethyl mustard oil"
3009 .... *alpha*-*3,3*-Trimethyl-*2*-norbornane methanol
1387 *1,3,3*-Trimethyl-*2*-norbornanol
1385 *1,3,3*-Trimethyl-*2*-norbornanone
1386 *1,3,3*-Trimethyl-*2*-norbornanyl acetate
1956 *3,6,7*-Trimethyl-*2,6*-octadienal
2096 *3,6,7*-Trimethyl-*1,6*-octadien-*3*-ol
2035 *3,6,7*-Trimethyl-*2,6*-octadienol
1958 *3,6,7*-Trimethyl-*6*-octenal
1960 *3,6,7*-Trimethyl-*6*-octenol
3010 .... *5,7,7*-Trimethyl-*2*-octenyl nitrile
1383 *6,10,14*-Trimethyl-*3,5,9,13*-pentadecatetraen-*3*-one
1382 *6,10,14*-Trimethyl-*5,9,13*-pentadecatrien-*2*-one
2994 *2,4,5*-Trimethyl phenylcyanide
2994 *2,4,6*-Trimethyl phenylcyanide
2003 *alpha*-*alpha*-*para*-Trimethyl phenylethyl alcohol
405 Trimethyl phenylmethane
3002 *2,4,6*-Trimethyl tetrahydrobenzalacetone
3002 *2,5,6*-Trimethyl tetrahydrobenzalacetone
3011 .... *2,6,6*-Trimethyl-*1,2,3,4*-tetrahydro benzalacetone
3000 *2,2,4*-Trimethyl-*1,2,5,6*-tetrahydrobenzaldehyde diethyl acetal
3012 *3,4,4*-Trimethyl-*1,2,3,4*-tetrahydronaphthalone
3012 .... *1,1,2*-Trimethyl tetralone-*3*
2764 *2,6,12*-Trimethyl trideca-*2,6,8*-trien-*10*-one
3015 Trimethyl undecanal
2766 *2,6,9*-Trimethyl undeca-*3,5,9*-trien-*10*-one
2014 *2,6,10*-Trimethyl-9-undecen-*1*-al
3013 .... *2,6,10*-Trimethyl-9-undecen-*1*-ol
3014 .... Trimethyl undecylenic aldehyde
3015 .... *2,6,10*-Trimethyl undecylic aldehyde
2809 *2,6,6*-Trimethyl-*2*-vinyl tetrahydropyran (see also 3016)
3016 .... *2,6,6*-Trimethyl-*6*-vinyl tetrahydropyran
558 *1,3,7*-Trimethyl xanthine
3017 .... Trinitro-*tertiary*-butyltoluene
3017 *2,4,6*-Trinitro-*3*-*tertiary*-butyltoluene
2282 *1,3,5*-Trinitro-*2*-*tertiary*-butylxylene
2282 *2,4,6*-Trinitro-*5*-*tertiary*-butyl-*meta*-xylene
2282 *2,4,6*-Trinitro-*1,3*-dimethyl-*5*-*tertiary*-butylbenzene
3017 *1,3,5*-Trinitro-*4*-pseudo-butyltoluene
887 Tri-*iso*-propylbenzaldehyde
2852 Trisodium citrate
2980 Tritolyl phosphate
3018 .... Tuberol (see also 926 and 1108)
3019 .... Tuberone
928 Tuberyl acetate
926 Tuberyl alcohol (see also 1108)
929 Tuberyl benzoate
2635 Tween
1761 Tyrosol
1885 Tyrosol methylether

U

245 "Umbellic acid"
3020 .... Umbelliferone
2255 Umbelliferone methylether
3021 Umbellularia californica
3021 .... Umbellulone
3022 .... Undeca-*2,4*-dien-*1*-al
3023 .... *2,3*-Undecadione
3024 .... *gamma*-Undecalactone
3025 .... *delta*-Undecalactone
3028 Undecaldehyde
3026 .... Undecamethylene carbonate
3026 Undecamethylene carboxylate
3027 .... Undecamethylene oxalate
3028 .... Undecanal
3029 .... Undecanal diethyl acetal
3030 .... Undecanal dimethyl acetal
3047 Undecanoic acetate
3051 Undecanoic acid
3050 Undecanoic formate
3031 .... Undecanol-*1*
2137 *n*-Undecanol-*2*

2138 *n*-Undecanol-*2*-acetate (see also 3047)
1523 *alpha*-Undecanolide-(*1:4*)
3024 Undecanolide-*1:4*
3025 Undecanolide-*1:5*
2140 *2*-Undecanone
1319 *3*-Undecanone
2715 *4*-Undecanone
467 *5*-Undecanone
877 *6*-Undecanone
3032 .... Undecatriene-*1,3,5*
3032 Undeca-*1,3,5*-triene
3033 .... *2*-Undecen-*1*-al
3033 *trans*-Undecen-*2*-al
3036 *cis-8*-Undecen-*1*-al
3034 .... *9*-Undecenal (see also 3033)
3034 *9*-Undecen-*1*-al
3036 *cis-9*-Undecen-*1*-al
3035 .... *10*-Undecen-*1*-al
3036 .... Undecenal, mxed isomers
3037 .... Undecenal diethyl acetal
3049 *9*-Undecene-*1*-carboxylic acid
3049 *9*-Undecenoic acid
3049 *10*-Undecenoic acid
3039 *n*-Undecenoic alcohol
3035 *n*-Undecenoic aldehyde
3040 *1*-Undecen-*10*-ol
3038 .... *2*-Undecen-*1*-ol
3039 Undecen-*1*-ol-*11*
3039 *9*-Undecen-*1*-ol
3039 .... *10*-Undecen-*1*-ol
3039 Undecen-*10*-ol-*1*
3040 .... Undecenol, mixed isomers
2078 "Undecenolide-*1:5*"
2427 *3*-Undecen-*2*-one
3041 .... Undecenyl acetate
3039 *9*-Undecen-*1*-yl acetate
3041 *10*-Undecen-*1*-yl acetate
3039 Undecenyl alcohol
3042 .... Undecenyl-*iso*-butyrate
3042 *10*-Undecen-*1*-yl-*iso*-butyrate
3048 Undecenyl butyrolactone
3043 .... Undecenyl formate
3043 *10*-Undecen-*1*-yl formate
3044 *10*-Undecen-*1*-yl heptanoate
3044 .... Undecenyl heptoate
3044 *omega*-Undecenyl heptylate
1564 Undecenyl heptylether
3045 .... Undecenyl phenylacetate
3046 *10*-Undecen-*1*-yl propanoate
3046 .... Undecenyl propionate
3046 *10*-Undecen-*1*-yl-*alpha*-toluate
3047 .... Undecyl acetate
2138 *secondary*-Undecyl acetate
3031 Undecyl alcohol
3028 Undecyl aldehyde
3029 Undecyl aldehyde diethyl acetal
3048 .... *alpha-n*-Undecyl-*gamma*-butyrolactone
1108 Undecyl carbinol
1121 Undecyl cyanide
3041 Undecylenic acetate
3049 .... Undecylenic acid
3039 Undecylenic alcohol
3034 Undecylenic aldehyde (see also 3035)
3036 Undecylenic aldehyde "internal isomers"
3037 Undecylenic aldehyde diethyl acetal
3050 .... Undecyl formate
1567 Undecyl heptylether
3051 .... Undecylic acid
3031 Undecylic alcohol
2137 *secondary*-Undecylic alcohol
3028 *n*-Undecylic aldehyde
3030 Undecylic aldehyde dimethyl acetal
3024 Undecyllactone
1523 *alpha-n*-Undecyllactone
839 Undecyl nitrile

V

2382 Valencene
3052 Valeral
3053 *iso*-Valeral
3052 .... *n*-Valeraldehyde
3053 .... *iso*-Valeraldehyde
3054 .... Valeraldehyde diamyl acetal
3055 .... *iso*-Valeraldehyde phenylethyleneglycol acetal
3056 Valerianic acid
3056 .... *n*-Valeric acid
3057 .... *iso*-Valeric acid
1941 *iso*-Valeric acid, optically active
2537 *active*-Valeric acid, phenylethyl ester
3052 *n*-Valeric aldehyde
3058 .... *iso*-Valeric anhydride
3059 .... *gamma*-Valerolactone
3059 *3*-Valerolactone
886 Valerone
480 *iso*-Valerone
3060 .... Valerophenone
3061 .... *iso*-Valerophenone
47 Valeryl acetyl
2841 *6*-Valeryl cyclohex-*1*-ene-*1*-carboxylic acid
3062 .... Valeryldinitro-*tertiary*-butyl-*meta*-xylene
3059 *gamma*-Valeryllactone
3063 .... *3-iso*-Validene-*2a,4*-dihydrophthalide
3064 .... *3-iso*-Validene phthalide
1854 "Validol"
3065 .... Valine
1899 *dl-iso*-Valine
2971 "Vanay"
1363 "Vanillal
3074 Vanillal acetone-(*1,3,4*)
1363 "Vanillarom"
3066 .... Vanillic acid
3076 Vanillic acid, vanillylester
3067 "Vanillic aldehyde"
1363 "Vanillidine"
3067 .... Vanillin
3068 .... *iso*-Vanillin
1888 *ortho*-Vanillin
50 Vanillinacetate dimethyl acetal
3075 "Vanillin diacetate"
3069 .... Vanillin ethylcarbonate-*para*-phenetidine
3070 .... Vanillin methylanthranilate
3077 Vanillin methylether
3069 Vanillin-*para*-phenetidine ethylcarboxylate

3071 .... Vanillin triacetate
1363 "Vanilllodin"
1363 "Vanillodor"
1363 "Vanillose"
1363 "Vanillum"
3072 .... Vanillyl acetate
3101 Vanillyl acetone
3073 .... Vanillyl alcohol
3074 .... Vanillylidene acetone
3075 .... Vanillylidene diacetate
3076 .... Vanillyl vanillate
1363 "Vanirom"
1363 "Vanirone"
1363 "Vanisol"
2646 "Vanitrope"
3008 "Vanoris"
1831 "Veltol"
1745 "Veltol plus"
3002 "Velvetine"
2091 "Velvione"
3077 .... Veratraldehyde
3077 Veratric acid
3077 *para*-Veratric aldehyde
3078 .... Veratrol
3079 .... Verbenone
1604 "Verdalol"
1799 "Verdanthiol"
432 "Verdol"
438 "Verdol acetate"
966 "Verdyl acetate"
435 "Verdone"
434 "*iso*-Verdone"
2208 "Verdoracine"
1608 "Verdural extra"
3080 .... Versalide
1696 "Vert de fleurs" (see also 2954)
2485 "Vert de lilas"
181 "Vert de violette" (see also 2045)
440 "Vertenex"
441 "Vertenex HC"
441 "Vertenex intercis"
2485 "Vertifol"
2485 "Vertodor"
3082 "Vetacetia"
3082 "Vetacetyl"
440 "Vetester"
3082 "Vetiriax"
1052 Vetivalene
3081 Vetivenol
3082 Vetivenol acetate
3083 Vetivenol butyrate
3083 Vetivenol-*iso*-butyrate
3085 Vetivenol formate
3084 Vetivenol octylate
3086 Vetivenol phenylacetate
3087 Vetivenol propionate
3088 Vetivenol valerianate
3082 Vetiver acetate
3081 .... Vetiverol
3089 Vetiverone
3082 .... Vetiveryl acetate
3083 .... Vetiveryl butyrate
3084 .... Vetiveryl caprylate
3085 .... Vetiveryl formate
3084 Vetiveryl octanoate
3084 Vetiveryl octoate
3086 .... Vetiveryl phenylacetate
3087 .... Vetiveryl propionate
3086 Vetiveryl-*alpha*-toluate
3088 .... Vetiveryl valerate
3088 Vetiveryl-*iso*-valerate
3081 Vetivol
3089 .... Vetivone (see also 1052)
3089 *alpha*-Vetivone
3089 *beta*-Vetivone
2273 "Vetsin"
3082 "Vetynal"
1137 "Vinegar naphtha"
3090 .... Vinyl acetate
73 Vinyl acetonitrile
2865 Vinyl benzene
63 Vinyl carbinyl acetate
64 Vinyl carbinyl anthranilate
65 Vinyl carbinyl benzoate
67 Vinyl carbinyl butyrate
72 Vinyl carbinyl cinnamate
69 Vinyl carbinyl decanoate
3091 .... Vinyl catechol carbonate
1891 *para*-Vinylcatechol-*ortho*-methylether
3094 *4*-Vinylcatechol-*1*-methylether
3092 .... *4*-Vinyl cyclohexene
868 Vinyl decyl ether
2454 Vinyl ethyl carbinol
2455 Vinyl ethyl carbinyl acetate
3093 .... Vinyl ethyl ether
53 Vinylformic acid
1462 Vinyl geranyl ether
1891 *para*-Vinylguaiacol
3094 .... *5*-Vinylguaiacol
1687 Vinyl hexyl carbinol
2359 Vinyl hexyl carbinyl acetate
2269 Vinyl methyl ketone
2608 Vinyl phenylacetate
2496 Vinyl phenyl carbinol
2495 Vinyl phenyl carbinyl acetate
2559 Vinyl phenylethyl ether
3095 .... Vinyl sulfide
827 "Violaron"
758 "Violet alpine"
2341 "Violet leaf alcohol" (see also 1010)
2339 "Violet leaf aldehyde"
2485 "Viridine"
932 "Virisacetal"
931 "Virisal"
572 Vitamin A (Provitamin A)
2243 Vitamin B-*1*
266 Vitamin C
2614 Vitamin E (see also 2613)

**W**
2241 Wintergreen oil, synthetic
1898 Wood alcohol
1898 Wood spirits
2780 Wood vinegar

**X**
1741 Xanthoxylin (see also 981)
981 *iso*-Xanthoxylin
1077 Xenene
3096 .... Xylene
3096 *meta*-Xylene
3096 *ortho*-Xylene

3096 *para*-Xylene
3097 .... *ortho*-Xylene oxide
3098 .... Xylenol
3098 *asymmetric-meta*-Xylenol
3098 *asymmetric-ortho*-Xylenol
3098 *meta-2*-Xylenol
3098 *meta-4*-Xylenol
3098 *meta-5*-Xylenol
3098 *ortho-3*-Xylenol
3098 *ortho-4*-Xylenol
3098 *para*-Xylenol
3098 *symmetric-meta*-Xylenol
3098 *vicinal-meta*-Xylenol
3098 *vicinal-ortho*-Xylenol
3098 *2,3*-Xylenol
3098 *2,4*-Xylenol
3098 *2,5*-Xylenol
3098 *2,6*-Xylenol
3098 *3,4*-Xylenol
3098 *3,5*-Xylenol
1039 *meta-4*-Xylenol allyl ether
266 *L*-Xyloascorbic acid
2282 Xylol moskus
2796 Xyloresorcinol
3099 .... Xylyl aldehyde
987 *2,4*-Xylyl aldehyde
3100 .... *beta-meta*-Xylyl ethanol
3100 *beta-meta*-Xylyl ethylalcohol
3097 *ortho*-Xylyl oxide

**Y**

2302 Yara-Yara
440 "Ylanat"
2346 "Ysminia"

**Z**

1463 Zdravetz
2273 "Zest"
2917 "Zibethal"
2917 "Zibethine"
3101 .... Zingerone
3102 .... Zingiberene

# Literature references

The last entry under the monograph of a chemical in this work is the literature reference.

All books, periodicals, data sheets, etc. used as literature reference have a number assigned to them, so that e.g.

66-710; means:

E. H. Rodd: Chemistry of Carbon Compounds, volume I, *page 710* (Elsevier, Amsterdam 1951-52).

and 90-806; means:

E. Gildemeister & Fr. Hoffmann: Die Ätherischen Öle, Band III d, *page 806,* (Akademie-Verlag, Berlin, 1966).

the first number in the reference indicating the book number in the following list, the second number indicating the page in the book.

Literature search for information to this work has been carried out since 1935 and the last entry was made in January 1969.

During these 34 years, many works have been omitted from the literature as outdated or superseded by newer, more correct sources of information. This explains the absence of many numbers in the literature reference list.

BEILSTEIN's Handbook of Organic Chemistry is referred to as

B-(volume No.)-(page No.). e.g. B-VII-416; means:

Beilstein, volume seven, page 416. The use of supplementary volumes is also indicated in the reference.

# Literature references

1: P. Karrer: Lehrbuch der Organischen Chemie, V' Aufl., Leipzig 1937.

3: Arno Müller: Internationaler Riechstoff-Kode II, 1942, Verlag Alfred Hüthig, Heidelberg.

4: Arno Müller: Internationaler Riechstoff-Kodex III, 1950. (A. Hüthig).

5: West, Strausz & Barton: Synthetic Perfumes, Their Chemistry and Preparation. London 1949, Edw. Arnold & Co.

6: Fr. Heusler: Die Terpene, 1896 (Friedr. Vieweg & Sohn, Braunschweig).

7: William A. Poucher: Perfumes, Cosmetics and Soaps, I, London 1941.

8: William A. Poucher: Perfumes, Cosmetics and Soaps, II, London 1941.

9: Schimmel's Berichte, 1942/43, Leipzig.

10: Schimmel's Berichte, 1944/47, Leipzig.

11: Variochem VVB Schimmel's Berichte 1948, Leipzig.

12: Variochem VVB Schimmel's Berichte 1950, Leipzig.

13: Organa VVB Schimmel's Berichte, 1951, Leipzig.

17: Miltizer Berichte der VVB Chemische Fabrik Miltiz, 1956.

26: Lange: Handbook of Chemistry, Ninth Edition, Ohio, U.S.A. 1956.

28: Hugo Janistyn: Riechstoffe, Seifen, Kosmetika, Vol. I, Heidelberg 1950.

30: R.W. Moncrieff: The Chemical Senses, 2' Edit. 1951, Leonard Hill Ltd., London.

31: R.W. Moncrieff: The Chemistry of Perfumery Materials, 1949, Leonard Hill, Ltd. London.

32: Soap Perfumery & Cosmetics 1949 (vol. XXII), United Trade Press, Ltd. F.V. Wells, Editorial Director, London.

33: same, 1950, vol XXIII

34: same, 1951, vol. XXIV

35: same, 1952, vol. XXV

36: same, 1953, vol. XXVI

37: same, 1954, vol. XXVII

38: same, 1955, vol. XXVIII

39: same, 1956, vol. XXIX

40: same, 1957, vol. XXX

41: same, 1958, vol. XXXI

42: same, 1959, vol. XXXII

43: same, 1960, vol. XXXIII

44: same, 1961, vol. XXXIV

45: same, 1962, vol. XXXV

46: American Perfumer, 1949-I, vol. 53 (Moore Publishing Co.), U.S.A.
47: same, 1949-II, vol. 54
48: same, 1950-I, vol. 55
49: same, 1950-II, vol. 56
50: same, 1951-I, vol. 57
51: same, 1951-II, vol. 58
52: same, 1952-I, vol. 59
53: same, 1952-II, vol. 60
54: same, 1953-I, vol. 61
55: same, 1953-II, vol. 62
56: same, 1954-I, vol. 63
57: same, 1954-II, vol. 64
58: same, 1955, vol. 65-66
59: same, 1956, vol. 67-68
60: same, 1957, vol. 69-70
61: same, 1958, vol. 71-72
62: same, 1959, vol. 73-74
64: Lothar von Jaminet: Aetherische Öle, Riechstoffe, Riechdrogen, Hamburg 1949.
65: Ernest Guenther: The Essential Oils, vol. II, van Nostrand, New York 1949.
66: E.H. Rodd: Chemistry of Carbon Compounds, vol. IA-IB, Elsevier Publ. Co., Amsterdam 1951-1952.
67: E.H. Rodd: Chemistry of Carbon Compounds, vol. IIA-IIB, Elsevier, Amsterdam 1953.
68: E.H. Rodd: Chemistry of Carbon Compounds, vol. IIIA-IIIB, Elsevier, Amsterdam 1954-1956.
69: E.H. Rodd: Chemistry of Carbon Compounds, vol. IVA-IVB, Elsevier, Amsterdam 1957-1959.
70: E.H. Rodd: Chemistry of Carbon Compounds, vol. V., Elsevier, Amsterdam 1962.
71: Jasper C. Maruzzella, Ph.D.: The Germicidal Properties of Perfume oils and Perfumery Chemicals (Amer. Perfumer 77, Jan. 1962, pages 67-70).
72: G.-F. Jaubert: Parfums Comestibles, Paris 1899, 3rd edition.
77: Alfons M. Burger: Das Buch der Aromen, 2' Ausgabe, Wädenswil, Schweiz 1955.
80: Shulton Inc.: Technical Bulletin No. 101: Lignyl acetate.
81: Shulton Inc.: Technical Bulletins No. 5-6-7: Vanitrope.
82: The Dow Chemical Co.: Techn. Information sheets: Palatone, 5/1/1948.
83: The Dow Chemical Co.: Techn. Information sheets: Cyclotene, 5/1/1948.
(The above two materials are no longer manufactured by Dow Chem. Co. but they are, since Jan. 1969, manufactured by Glidden-Durkee Corp. U.S.A.).
85: Arno Müller: Die Physiologischen und Pharmakologischen Wirkungen der Ätherischen Öle, Riechstoffe und Verwandten Produkte, 2' Auflage, Alfred Hüthig, Heidelberg 1951.
86: Arno Müller: Internationaler Riechstoff-Kodex, Ergänzungsband 1957, dritter Auflage, Verlag Alfred Hüthig, Heidelberg.

87: E. Gildemeister/Fr. Hoffmann (W. Treibs und D. Merkel): Die Ätherischen Öle, Band IIIa, Akademie-Verlag, Berlin 1960.
88: same, Band IIIb, 1962.
89: same, Band IIIc, 1963.
90: same, Band IIId, 1966.
93: Ätherische Öle, Riechstoffe, Parfumerie, Essenzen und Aromen, July 1953, Berlin.
95: Georg Cohn: Die Riechstoffe, Verlag Friedr. Vieweg und Sohn, Braunschweig, 1924.
96: R. Knoll und A Wagner: Synthetische und Isolierte Riechstoffe, II'Auflage, Verlag Vilhelm Knapp, Halle 1928
100: Merck's Index, Seventh edition, Rahway 1960 (U S A ).
102: S. P. C. Yearbook 1958, United Trade Press Ltd., London.
103: Ed.S. Maurer: Perfumes and Their Production, United Trade Press Ltd., London 1958.
104: S. Arctander: Perfume and Flavor Materials of Natural Origin, S. Arctander. 1961. Elizabeth, N.J. (U.S A ).
105: G. Fenaroli: Sostanze Aromatiche Naturali, Ulrico Hoepli, Milano 1963.
106: The Givaudan Index, Second Edition, New York 1962 (U.S.A.).
107: J. Merory: Food Flavorings -. Avi Publishing Co. Westport, Conn. 1960 (U.S.A.).
113: Soap, Perfumery and Cosmetics, 1963, vol. XXXVI (United Trade Press Ltd.). F.V. Wells, Editorial Director, London.
114: same, 1964, vol. XXXVII
115: same, 1965, vol. XXXVIII
116: same, 1966, vol. XXXIX
117: American Perfumer and Cosmetics, vol. 75, 1960, Allured Publ. Corp. (U.S.A.).
118: same, vol. 76, 1961.
119: same, vol. 77, 1962.
120: same, vol. 78, 1963.
121: same, vol. 79, 1964.
122: same, vol. 80, 1965.
123: same, vol. 81, 1966.
124: Edw. P. Claus: Pharmacognosy, 1961. Leo & Fibiger, Philadelphia, U.S.A.
126: Wm.A. Poucher: Perfumes, Cosmetics & Soaps, vol. I, Sixth Edition 1959, Princeton, N.J. (U.S.A.).
127: same, vol. II, 1959.
130: Geo. Edw. Trease: A Textbook of Pharmacognosy, 8th Edit. 1961, Bailliere, Tindall and Cox, London.
132: Romuald Klimek: Oleiki Eteryczne, Warszawa 1957.
135: Vladimir Nikolayevitch Belov: Chemistry and Technology of Synthetic and Natural Odor Substances; All-Union Inst. of Syn. & Nat. Od. Subst., Moscow 1963 (in Russian).
140: Alfons M. Burger: Die Natürlichen und Künstlichen Aromen, Alfred Hüthig, Heidelberg 1968.

145: P.M. Jenner, E.C. Hagan, Jean M. Taylor, E.L. Cook & O.G. Fitzhugh: Acute Oral Toxicity (of 107 synthetic and natural flavourings and structurally related compounds), May 1964, Food and Drug Administration, United States Department of Health, Education and Welfare, Washington 25, DC, U.S.A. Pergamon Press (U.K.) 1964.
150: same – in Food & Cosmetics Toxicology, volume II, pages 327-343.
151: Chemicals Used in Food Processing, Publication No. 1274, National Research Council, Washington DC, U.S.A., 1965.
152: Flavor components in Food (a bibliography). Svenska Institutet för Konserveringsforskning 1965. Erik von Sydow and Madelaine Westberg.
153: G.R.A.S. substances. By Richard L. Hall and Bernard L. Oser. Printed in Food Technology, Febr. 1965, pages 151-197.
154: Food Chemicals Codex, November 1964 (and later). National Academy of Sciences, National Research Council, Washington DC, U.S.A.
155: Hugo Janistyn: Taschenbuch der Modernen Parfumerie und Kosmetik, Wissenschaftliche Verlagsgesellschaft mbH, Stuttgart 1966.
156: Paul Z. Bedoukian: Perfumery and Flavoring Synthetics, Elsevier 1967, Amsterdam & New York.
157: Chemistry & Physiology of Flavors (a Symposium on Foods). Schultz, Day and Libbey; Avi Publ. Co. Connecticut, U.S.A. 1967.
158: Flavor Chemistry (15 papers from a 1965 symposium in Detroit, Mich. U.S.A.) "Advances in Chemistry" series No. 56. American Chemical Society, Washington DC, 1966.
159: R.W. Moncrieff: The Chemical Senses, IIIrd edition 1967. Leonard Hill Ltd., London.
160: Handbook of Chemistry and Physics, 44th edition 1963. The Chemical Rubber Publishing Co., Cleveland Ohio, U.S.A.
161: J. Merory: Food Flavorings, The Avi Publishing Co., Westport, Conn. U.S.A., 1968.
162: E. Furia: Handbook of Food Chemicals. The Chemical Rubber Co., Cleveland, Ohio, U.S.A. 1968.
163: Arno Müller: Internationaler Riechstoff-Kodex, 4th edition 1968, Alfred Hüthig Verlag, Heidelberg.
164: R. Harper, E.C. Bate Smith & D.G. Land: Odour Description and Odour Classification. American Elsevier Publishing Co., New York 1968.
165: R.W. Moncrieff: Odour Preferences, 1966. The Grampian Press/Leonard Hill Ltd., London.

The Fritzsche Library Bulletin (Dr. R.T. Koenig, Editor) has been extremely useful and time-saving in the author's search for additional information on various subjects treated in this work.